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ADDITION TO THE LEWIS CHEMICAL EQUILIBRIUM PROGRAM TO ALLOW COMPUTATION FROM COAL COMPOSITION DATA

DECEMBER, 1980

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COMPUTER SCIENCES CORPORATION

ADDITION TO THE LEWIS CHEMICAL EQUILIBRIUM PROGRAM TO ALLOW COMPUTATION FROM COAL COMPOSITION DATA

DECEMBER, 1980

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1.0 INTRODUCTION

This document reports changes made to the Lewis Chemical Equilibrium Program in order to adapt it for use by the Coal Gasification Project. The program was developed by the Lewis Research Center for analysis of the chemical equilibrium combustion in rocket engines. It can be applied directly to the entrained flow coal gasification process. The particular problem addressed is the reduction of the coal data into a form suitable to the program, since the manual process is involved and error prone. A similar problem in relating the normal output of the program to parameters meaningful to the coal gasification process was also addressed.

The revisions included in this writeup act as buffers on both sides of the Lewis Chemical Equilibrium Program to allow direct processing of raw coal gasification data and the production of data meaningful in coal gasification terms.

This document includes a Program Task Description of the capabilities created by the revisions of the original program. A list is given for the program elements which have been altered. Also included are two sample problems and a printout of the original program with and without the modifications for processing of coal gasification data.

The work was performed for the Engineering Systems Branch (AH33) of the Computer Services Office under contract NAS8-31640. The sponsoring organization was the Coal Gasification Task Team (PF15).

1.1 References

This program is self-contained and requires no other documents for its use and execution. Included for clarification are a memo by David Seymour, "Application of Lewis Chemical Equilibrium Computer Program to Coal Gasification" in Appendix A (Reference 2). If further revisions of this program become necessary, consult the "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shock, and Chapman - Jouget Detonation" by Gordon and McBride, NASA SP-273 (Appendix B, Reference 1).

2.0 PROGRAM TASK DESCRIPTION

The Lewis Chemical Equilibrium Program was revised to include the following capabilities:

1. Accept data in the form of coal and other fuel element compositions and create reactant data compatible with the original program.
2. Store and edit the coal composition data.
3. Increase the number of elements within a compound from four to five.
4. Increase the number of reactants in the system from 15 to 25.
5. Provide a means of removing certain species from consideration during coal calculations.
6. Provide for coal data only, that input temperatures be in °F and that printout of pressure, temperature, enthalpy and entropy be in English units.
7. Provide, for coal data only, an additional section of output listing.
8. Allow the use of a new pseudo element, inert carbon.
9. Provide a store and edit feature for namelist list.
10. Provide that types of input data, as represented by various menu items, be enterable in any order.
11. Simplify loading the program onto the terminal.
12. Provide a simple means of creating a copy of the system tape with the data from the previous run.

The program which provided the base for the revisions was "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shock, and Chapman-Jouget Detonation" by Gordon and McBride, NASA SP-273. This program had been previously revised to provide interactive input and output via the Marshall Interactive Planning System (MIPS).

A complete listing of the source code is appended so that the changes indicated in the Revisions section may be followed.

3.0 REVISIONS OF LEWIS CHEMICAL EQUILIBRIUM PROGRAM

The current revision is discussed in relation to the changes required in various subroutines and how they relate to the new capabilities. Also discussed are the new inputs and outputs required or generated by the revision. Finally, a complete sample case, for coal data, is presented.

3.1 Storage Element A (Map overlay source code)

A new segment COALCV was added to handle the conversion of coal data to reactant data. Note that this segment is the longest and may at some future time have to be split into more segments.

3.2 Storage Element BLOCK1 (Miscellaneous data - Block data form)

The entry for atomic weight and valence of Deuterium was replaced with the atomic weight and valence of the pseudo element, inert carbon. The element symbol is IC and the weight and valence are those of regular carbon. The inert carbon element is used in the simulation of coal gasifier systems which have an unreacted carbon recycle stream.

3.3 Storage Element BOOT (Bootstrap control section)

The control statements serve to assign, copy and catalog the five files necessary to run the program. The catalog is included to insure that additional runs made on the same day do not have to reload the tape.

Note that BOOT is part of the first file on the system tape for the program. The following control statements are necessary to load the complete system:

```
@ASG,T PUR,U9S,XXXXX
@COPY,G PUR.TPF$.
@ADD TPF$.BOOT
```

The first part of Sample 1 shows the complete loading process.

File LEWIS contains all the subroutines and map elements. File 4 contains the thermodynamic data. Files 8, 10, and 12 contain dummy reactant data, namelist data and coal data, respectively.

3.4 Storage Element CHECK (Subroutine CHECK)

No changes.

3.5 Storage Element COALCV (Subroutine COALCV)

The subroutine COALCV is a new subroutine designed to do the major processing of converting coal composition data to reactant data.

The appended memo "Application of the Lewis Chemical Equilibrium Computer Program to Coal Gasification" by David C. Seymour (A-1) discusses the detailed calculations to be made based on the input data.

The subroutine assumes the existence of a previous set of coal data, stored in file 12. A set of coal reactant data immediately follows the coal data on file 12. This data is in the same form as the reactant data written by subroutine RREAD for data which is entered in the normal fashion. A dummy set of coal data is provided as part of the system tape. The user is queried as to whether he wants a printout of the previous data set. A response of YES produces a listing of the original coal data in the form shown in Sample 2. Regardless of whether a printout of the past data is requested, the past data is always read except for the conditions of first pass and no request for past data.

Table 1 explains the variables used by COALCV to store the coal data and the record groupings of the data. Table 2 explains the various possible measured or empirical values of higher heating value.

After printing the existing data, the user is prompted as to whether he wishes to modify the data, add to the data or continue with the same data. For the continue option, the subroutine exits. For the modify flag, a further prompt is given requesting the data group numbers of the data to be changed. See the last line of Sample 1. Each data group has associated with it a flag which indicates whether that type of data is to be processed. For the modify option, the flags of only those groups requested are turned on. For the add option, all flags are turned on.

Each data group flag is queried. If the flag is on, appropriate prompts are issued and the resulting information as entered by the user is stored in the appropriate variable. Two of the data groups, ash and other fuels, have additional special processing. For those data groups, two paths are possible. If the modify option was chosen, then it is possible to modify, delete or add individual lines to the existing material, via a series of prompts and responses. If the modify option was not chosen, the prompts and responses insert a completely new set of data.

Note that for ash composition, four of the common compounds are prompted for individually. If the weight of any of these is returned as 0 (or blank), that compound is eliminated. Note also that for other fuels, a search is made to determine which fuel number corresponds to water so that the proper water to coal ratio may be computed.

When all the required data groups have been entered, then the calculations outlined in the included paper are done, except for the section "Use and Interpretation of CEC Results". That section is done in another subroutine.

The coal data is saved on file 12 followed by the computed reactant data. The coal data is in the form shown in Table 1. The reactant data is in the same format as for the original program, except that the first record contains the coal to fuel ratio (CF) in addition to the number of reactants (NREAC). The subroutine then returns to the calling routine.

TABLE 1

COALCV VARIABLES

Record 1	
NREAC	Number of reactants
CF	Coal to fuel ratio
HHVV	Higher heating value of coal Btu/lb
WCR	Water to coal ratio
PER	Fraction carbon conversion
Record 2	
CTEMP	Coal temperature (°F)
OTEMP	Oxidizer Temperature (°F)
Record 3	
PROX(3)	Proximate Analysis volatiles, fixed carbon, ash
COAL(5,2)	Coal composition in form element and number in order C, H, N, O, S.
PER	As above in record 2
IE	Pointer to higher heating value table
HH(8)	Measured and empirical higher heating value table. See table 2 for possible values.
Record 4	
NCOAL	Number of other coal elements, other than C, H, N, O, S.
NASH	Number of ash compounds
NFUEL	Number of fuel compounds other than coal.
NOXID	Number of oxidizer compounds.
Record 5*	
CCOMP(12,5)	Other coal components in the form, weight, percent, state, and compound.
ACOMP(11,8)	Ash components in the form, weight percent and compound.
OFUEL(13,8)	Other fuel components in the form, weight, percent, temperature, state and compound.
OXID(11,5)	Oxidizer components in the form, weight percent and compound.

*Compound in this section indicates that a chemical compound is broken down into its component atoms and number of atoms. That is: $CaCO_3$ = Ca 1.0 C 1.0 0 3.0

TABLE 2

Possible Higher Heating Values

1 Measured Data

2 Dulong 1

$145.44(\%C) + 620.28(\%H - 1/8(\%O)) + 40.5(\%S)$

3 Dulong 2

$146.0(\%C) + 620.0(\%H-1/8(\%O)) + 40.5(\%S)$

4 CPP2

$144.9(\%C) + 610.0(\%H-1/8(\%O)) + 55.5(\%S)$

5 Grummel and Davis

$$\left[\frac{654.3(\%H)}{100. - \%Ash)} + 424.62\right] \left[\frac{\%C}{3} + \%H - \frac{\%O}{8} + \frac{\%S}{8}\right]$$

6 Coal Conversion System Technical Data Base (CCSTDB)

$146.58(\%C) + 568.78(\%H) + 29.4(\%S)$
$- 6.58(\%Ash) - 51.53(\%O + \%N)$

7 Maximum of 2 through 6

8 Minimum of 2 through 6

3.6 Storage Element CPHS (Subroutine CPHS)

Changes were made in the COMMON area MISC to accommodate 25 instead of 15 reactants. The variables changed were LLMT, B0, BOP, DATA, NAME (first dimension), ANUM (first dimension) PECWT, ENTH, FAZ, RTEMP, DENS, and RMW. In addition, the dimension of NAME (second dimension) and ANUM (second dimension) were changed to accommodate 5 elements within a compound rather than 4. Note that the last column of the array is used to store a flag indicating whether or not the enthalpy of the reactant is to be calculated.

3.7 Storage Element DETON (Subroutine DETON)

Same changes as for CPHS.

3.8 Storage Element EQLBRM (Subroutine EQLBRM)

Same changes as for CPHS.

Also increased temporary storage PROW to 25 from 15.

Added a temperature condition to the error message which states that "100 iterations did not satisfy the convergence requirement".

3.9 Storage Element FROZEN (Subroutine FROZEN)

Same changes as for CPHS.

3.10 Storage Element GAMEFF (Subroutine GAMEFF)

No changes.

3.11 Storage Element GAUSS (Subroutine GAUSS)

No changes.

3.12 Storage Element HCALC (Subroutine HCALC)

Same changes as for CPHS.

In addition the temporary storage area NUM was redimensioned 25 x 6. All references to NAM (N,5) or NAME (N,5) were changed to(N,6). All array processing of ANUM was increased by 1.

3.13 Storage Element LTCPHS (Subroutine LTCPHS)

No changes.

3.14 Storage Element MAIN (Subroutine MAIN - system driver)

Same changes as for CPHS in the data area. Also the addition of COMMON area CFUEL and the addition of a data area (NOMTS) which represent those species which can be eliminated from consideration when working with coal data. See Table 3 for a summary of the species. The upper limit of 150 possible species is often exceeded when using coal data. The optional omission species can be used to remove some of the least likely possibilities.

In the body of the subroutine the value of CF is initialized to -1.0. If CF remains as -1.0, then the coal data section was never entered since that section will produce a positive value of CF. The CF flag is used in other subroutines to initiate action required by the presence of coal data.

All the entries in namelist, INPT2, are initialized.

The menu of possible choices was expanded by addition of Item 7, 'start program calculation' and Item 8, 'insert or edit coal data.' The wording of Items 1 to 6 were reworked to make them consistent.

A request for Item 8 produces a call to subroutine COALCV and processing returns to the menu list. For menu Item 3, the call is made to subroutine RREAD rather than to subroutine REACT. This is to make the data entry independent of order. The decision on logical flag CALCH was moved to menu Item 7. In the move, references to NAME (N,5) were replaced with (N,6).

Menu Items 4 and 5 were corrected to properly store the species name being placed in the omit and insert lists.

Menu Item 6, concerning namelist, had an edit feature added. A dummy namelist is stored by the system on File 10. The user is queried as to whether he wishes to see the previous namelist. A response of YES prints the previous list and then the user is asked whether he wishes to change the namelist. The program either stops for new namelist data or returns to the menu list. A response of NO in the print namelist question, totally initializes the namelist and then stops to input new items. Return is to the menu list.

TABLE 3

Optional Omission Species

AL(S)
AL(L)
AL CL2
ALN(S)
ALN
C
C3
C4
C5
H20(S)
03
SI
SIC
SIC2

SI(S)
SI(L)
SICL
SICL2
SICL3
SICL4
SIH
SIH4
SIN
SI2
SI20
SI2N
SI3

Menu Item 7 was added to separate Item 6 from the actual start of the program so that Menu Items 1-6 and 8 can be input in any order. The new section moves the printout of the final namelist from Menu Item 6, the determination of logical CALCH from Menu Item 3 and the initialization of RHOP, VOL and NT from the original initialization area. In addition, this section requests the omission of the special coal data omit candidates.

Some special processing of Menu Item 7 is required by the exclusion of coal data. If the fraction of carbon conversion (PER) is less than 1, the special inert carbon element must be placed in the insert list. If the logical flag ERATIO is false and flag CF is positive then all MIX values must be multiplied by CF. MIX supposedly represents oxidizer to fuel ratio. For coal data, it is more convenient to input oxidizer to fuel ratio. The internally calculated coal to fuel ratio (CF) is then used to adjust to the proper O/F ratio. Also all namelist temperatures read in °F when coal data is being used, are adjusted to °K.

3.15 Storage Element MATRIX (Subroutine MATRIX)

Same changes as for CPHS.

3.16 Storage Element OUT1 (Subroutine OUT1 entries OUT2, OUT3, OUT4)

Same changes as for CPHS.

In addition, for coal data only, an additional line is printed at the end of the OUT1 printout. The line identifies oxidizer/coal ratio, water/coal ratio and fraction carbon conversion.

In the OUT2 section, for coal data only, pressures are printed in lbs per square inches, temperatures in °F, enthalpy in Btu/lb, entropy in Btu/(lb °F), and density in lb./cu.ft. The program pauses at the end of OUT2 to produce hardcopy of the output.

In the OUT3 section, for coal data only, an extra header line is printed. It is exactly the same as the line printed by OUT1.

The OUT4 section is new and corresponds exactly to the section "Use and Interpolation of CEC Results."

Sample 3 shows the printout created by each section of OUT1.

3.17 Storage Element PROK (PDP Element PROK)

No changes.

3.18 Storage Element REACT (Subroutine REACT)

Same changes as for CPHS.

Addition of common area CFUEL. Dimension changes of temporary variables ANAME, V, LLMTS, SBOP changes to array processing to handle 25 instead of 15 reactants. Change array processing ANUM and NAME to handle extra element within reactant.

The call to subroutine RREAD was removed and placed in MAIN. REACT now creates the final reactant data arrays by adding reactants placed on the reactant file (4) by the normal reactant input and those coal data reactants which are stored on the coal data file (12). The subroutine uses a two pass system. The first pass reads the first record from the coal data file if CF is -1. This places necessary header data into the system. If any normal reactants exist, they are read into the appropriate data areas. When all the reactants are read, the coal data reactants are read and added to the appropriate data areas.

3.19 Storage Element RKTOUT (Subroutine RKTOUT)

Addition of COMMON area CFUEL.

A call to OUT4 if coal data is present.

3.20 Storage Element ROCKET (Subroutine ROCKET)

Same changes as in CPHS.

Added a prompt for namelist RKTINP.

3.21 Storage Element RREAD (Subroutine RREAD)

Temporary arrays NAME, ANUM, PECWT, MOLE, ENTH, FAZ, RTEMP, FOX, DENS were adjusted to handle 25 instead of 15 reactants. NAME and ANUM were also adjusted to handle an additional element within the reactant. Array processing of these arrays was adjusted accordingly. The COMMON area CFUEL was added.

The first record of the reactant file was amended to include the value of CF. The individual reactant lines were adjusted to isolate the code which indicates that the enthalpy should be calculated. Previously, it had been recorded as part of the NAME array.

In addition, the edit section was made two pass. In the first pass, the data which is added or edited, is placed on the reactant file. Data to be edited also comes from this file. On the second pass, if one is requested, it is taken from the coal reactant data portion of the coal data file. Updates and/or additions are made to this data and the changed data is returned to the coal data file behind the original coal data. Note that the reactant data from the two sources is not added together until subroutine REACT, which is part of the startup routine. The setting of flag FIRST was removed from subroutine RREAD.

3.22 Storage Element SAVE (Subroutine SAVE)

Same changes as for CPHS. Addition of COMMON area CFUEL.

Creation of an additional header line, for coal data only. The line contains oxidizer/coal ratio, water/coal ratio and fraction carbon conversion. This header occurs just before the summation of atoms in the system.. See Sample 2, labeled SAVE.

3.23 Storage Element SEARCH (Subroutine SEARCH)

Same changes as for CPHS. Added a specific number for number of species in system. Also added a pause at the end of the species printout to obtain a hardcopy.

3.24 Storage Element SHCK (Subroutine SHCK)

Same changes as for CPHS.

3.25 Storage Element TAPESAVE (Tape Save Control Section)

The control statements serve to assign a tape, called LEWISTAPE, and copy the five system files into the tape. The following statement is necessary to call the tapesave system:

```
@ADD LEWIS.TAPESAVE
```

3.26 Storage Element THERMP (Subroutine THERMP)

Same changes as for CPHS. Added COMMON area CFUEL.

Addition of a pause to create a hardcopy of the material prior to the output of THERMP.

For coal data only, a call to entry OUT4 of subroutine OUT1.

Also, a pause at the end of THERMP to create a hardcopy before the next data set is processed.

3.27 Storage Element VARFMT (Subroutine VARFMT)

No changes.

3.28 Thermodynamic Data (File 4)

Thermodynamic data for the pseudo element inert carbon was added to the data. The data was that for C(S) with the exception of the compound name and atom name.

4.0 SAMPLE PROBLEM 1

The following pages indicate the procedure to load the Lewis Chemical Equilibrium Program and input new coal data into the system.

The data set which is being illustrated is the same as in the attached memo (A-1).

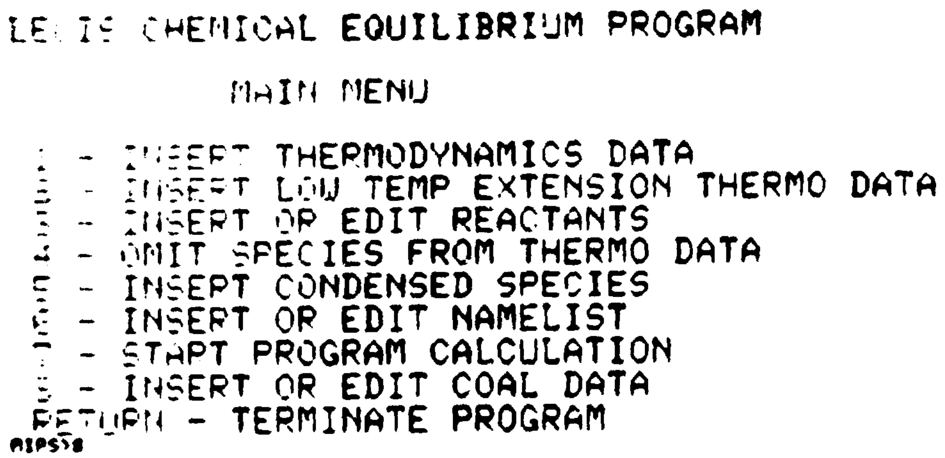
```
PORT 28/49  SIGNON  - HOST1(2X0) UP  HOST2(2X0) UP
RTYP04
ENTER USERID/PASSWORD
>PAYLOADS ESD


*DESTROY USERID/PASSWORD ENTRY
*UNIVAC 1100 OPERATING SYSTEM  LEV  AX30R2BHOST1(RSI)*
*************************************************************************************
>@RUN LEWIST 1HPD013X0000.SEVIGNBIN208.30.200
DATE  081880      TIME  094204
>@ASG,T PUP U9S.02130
READY
>@COPY,G PUP .TPF$
FURPUR 28R1H1 E36 S74T11 08/18/80 09.42.46
SEVIGNBIN208*LEWIS(1) COPIED ON 08/04/80 AT 14.23.18
   105 BLOCKS COPIED
EOF ENCOUNTERED ON INPUT TAPE
>@ADD  TPF$.BOOT
READY
READY
READY
READY
READY
READY
READY
READY
READY
READY
FURPUR 28R1H1 E36 S74T11 08/18/80 09.44.26
   105 BLOCKS COPIED
SEVIGNBIN208*4(1) COPIED ON 08/04/80 AT 14.24.49
    17 BLOCKS COPIED
EOF ENCOUNTERED ON INPUT TAPE
SEVIGNBIN208*8(1) COPIED ON 08/04/80 AT 14.25.17
     1 BLOCK  COPIED
EOF ENCOUNTERED ON INPUT TAPE
SEVIGNBIN208*10(1) COPIED ON 08/04/80 AT 14.25.30
     1 BLOCK  COPIED
EOF ENCOUNTERED ON INPUT TAPE
SEVIGNBIN208*12(1) COPIED ON 08/04/80 AT 14.25.49
     1 BLOCK  COPIED
EOF ENCOUNTERED ON INPUT TAPE
READY
>
```

ORIGINAL PAGE IS
OF POOR QUALITY

```
@MIPS.L
READY
FACILITY WARNING  100000000000
FILE HAS BEEN PREVIOUSLY ASSIGNED (OR FREED)
READY
FURPUR 28R1M1 E36 S74T11 08/21/80 08 11 07
 1 ABS
     12 BLOCKS COPIED
     12 BLOCKS COPIED
     64 BLOCKS COPIED
```

```
  MIPS INITIALIZATION IS IN PROGRESS
OFF-LINE MAINTENANCE PROCESSOR LAST RUN AT 08/18/80  09:17:37
 TOTAL SUP TIME =   2.17 MIN
SELECT NEW PRINT FILE OPTION:
1  - WRITE PRINT FILE ON PAPER
2  - WRITE PRINT FILE ON FICHE
MIPS>1
    A PRINT FILE HAS BEEN ESTABLISHED NAMED    MPS105551*P$F$.
 INSERT COMMANDS : (INSERT    HELP    FOR TUTORING)
MIPS>&XQT LEWIS B
MIPS>SV ONE
 SAVE COMPLETED
MIPS>RN ONE
MIPS>GO
```

```
TYPE YES  FOR PRINT TO PRINT FILE
[illegible]
```



```
LEWIS CHEMICAL EQUILIBRIUM PROGRAM

          MAIN MENU

 1 - INSERT THERMODYNAMICS DATA
 2 - INSERT LOW TEMP EXTENSION THERMO DATA
 3 - INSERT OR EDIT REACTANTS
 4 - OMIT SPECIES FROM THERMO DATA
 5 - INSERT CONDENSED SPECIES
 6 - INSERT OR EDIT NAMELIST
 7 - START PROGRAM CALCULATION
 8 - INSERT OR EDIT COAL DATA
 RETURN - TERMINATE PROGRAM
```

AIPS58

ORIGINAL PAGE IS
OF POOR QUALITY

```
TYPE YES TO READ IN PREVIOUS COMPOSITION
NIPS>NO
```

```
                                                                MIPS)
 TYPE (OPTIONAL) LBS VOLATILES/100 LBS DRY COAL
MIPS)37.54
 TYPE LBS ASH/100 LBS DRY COAL
MIPS)15.93
 TYPE COAL TEMPERATURE IN DEG F
MIPS)77
 TYPE LBS/100 LBS DRY COAL FOR ELEMENTS
 C
MIPS)67.31
 H
MIPS)4.757
 N
MIPS)1.529
 O
MIPS)6.343
 S
MIPS)4.1
 TYPE (OPTIONAL) OTHER COAL COMPONENTS
 TYPE LBS/100 LBS DRY COAL STATE AMD AND COMPONENT
 COAL TEMPERATURE IS ASSUMED
     EXAMPLE 0.13  1HG  2HCL  2
MIPS)0.13 1HG 2HCL 2
MIPS)
 TYPE LBS/100 LBS DRY ASH FOR COMPONENTS
 STATE ASSUMED SOLID  COAL TEMPERATURE ASSUMED
 SIO2
MIPS)52.69
 FE2O3
MIPS)26.08
 AL2O3
MIPS)20.23
 FES2
MIPS)
 CONTINUE WITH ASH COMPONENTS
 LBS/100 LBS DRY ASH AND COMPONENT
     EXAMPLE  0.25  2HTI  1   1HO  2
MIPS)
 TYPE CARBON CONVERSION FRACTION  FOR EXAMPLE. 0.89
MIPS)0.945
 HHV CALCULATION
 0 - ENTER DATA
 1 - DULONG 1          12414.484
 2 - DULONG 2          12451.067
 3 - CPP2              12398.885
 4 - GRUMMEL-DAVIS     12423.143
 5 - CCSTDB            12182.720
 6 - MAX OF ABOVE      12451.067
 7 - MIN OF ABOVE      12182.720
MIPS)0
 ENTER HHV AS BTU/LB COAL
MIPS)12141
 TYPE OTHER FUEL COMPONENTS
 TYPE LBS/LB COAL  TEMPERATURE (DEG F) AND STATE AND COMPONENT
     EXAMPLE  0.31  100   1HG  1HH  2   1HO  1
MIPS)0.1 212  1HG 1HH 2  1HO 1
MIPS)
 TYPE IN OXIDIZER TEMPERATURE. DEG F
MIPS)77
 TYPE OXIDIZER COMPONENTS
 TYPE LBS/100 LBS OXIDIZER AND COMPONENT
     EXAMPLE  95.0  1HO  2
MIPS)95  1HO 2
MIPS)5. 2HAR 1
```

```
 INDEX
                                     REACTANT(*)
                                                                           REL WT/    MOLE  ENTHALPY/       PHASE  TEMP.K    FUEL/  DENSITY
  1  C   49 7311  H  44 3187  N    1 0251  O    3 7243  S    1 2008   NO MOLES        INT ENERGY                    OXID
  2  IC   1 0000          0000         0000         0000         0000     730336   -222076 7500      S     298 150    F     00000
  3  CL   2 0000          0000         0000         0000         0000     033655          0000*      S     298 150    F     00000
  4  SI   1 0000  O   2 0000         0000         0000         0000     001182          0000*      G     298 150    F     00000
  5  FE   2 0000  O   3 0000         0000         0000         0000     077258          0000*      S     298 150    F     00000
  6  AL   2 0000  O   3 0000         0000         0000         0000     037535          0000*      S     298 150    F     00000
  7  H    2 0000  O   1 0000         0000         0000         0000     029116          0000*      S     298 150    F     00000
  8  O    2 0000          0000         0000         0000         0000     090909          0000*      G     373 150    F     00000
  9  AR   1 0000          0000         0000         0000         0000     950000          0000*      G     298 150    O     00000
                                                                      050000          0000*      G     298 150    O     00000
  TYPE  1  2 OR 3  TO MODIFY, DELETE, OR ADD A REACTANT      *      INDICATES ENTHALPY TO BE CALCULATED
MIPS>                                                  (RETURN TO CONTINUE)
TYPE YES FOR SPECIAL OMITS FOR COAL DATA
MIPS>YES
```

```
LEWIS CHEMICAL EQUILIBRIUM PROGRAM

          MAIN MENU

 1 - INSERT THERMODYNAMICS DATA
 2 - INSERT LOW TEMP EXTENSION THERMO DATA
 3 - INSERT OR EDIT REACTANTS
 4 - OMIT SPECIES FROM THERMO DATA
 5 - INSERT CONDENSED SPECIES
 6 - INSERT OR EDIT NAMELIST
 7 - START PROGRAM CALCULATION
 8 - INSERT OR EDIT COAL DATA
 RETURN - TERMINATE PROGRAM
```

MIPS76

```
TYPE YES FOR PRINT INPT2 NAMELIST
MIPS> NO
 BEGIN NAMELIST INPT2 INPUT
> $INPT2 MIX= 9, P=15  $END
```

ORIGINAL PAGE IS
OF POOR QUALITY

```
$INPT2
DETN      •  F
ERATIO    •  F
FA        •  F
FPCT      •  F
HP        •  T
IDEBUG    •                +0
IONS      •  F
MIX       •      91000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00
MMHG      •  F
NSQM      •  F
OF        •  T
P         •      15000000E+02.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00
PSIA      •  T
RKT       •  F
S0        •      00000000E+00
SHOCK     •  F
SO        •      00000000E+00
SP        •  F
SU        •  F
T         •      00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+06.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00
TP        •  F
TU        •  F
UU        •  F
V         •      00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00.     00000000E+00.     00000000E+00.     00000000E+00.
                 00000000E+00

$END




READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
MIPS>
```

```
LEWIS CHEMICAL EQUILIBRIUM PROGRAM

          MAIN MENU

 1 - INSERT THERMODYNAMICS DATA
 2 - INSERT LOW TEMP EXTENSION THERMO DATA
 3 - INSERT OR EDIT REACTANTS
 4 - OMIT SPECIES FROM THERMO DATA
 5 - INSERT CONDENSED SPECIES
 6 - INSERT OR EDIT NAMELIST
 7 - START PROGRAM CALCULATION
 8 - INSERT OR EDIT COAL DATA
 RETURN - TERMINATE PROGRAM
MIPS>7
```

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```
SPECIES BEING CONSIDERED IN THIS SYSTEM
    J12/65  AL           J 6/70  ALCL         J 6/70  ALCL3(S)     J 6/70  ALCL3(L)     J 6/73  ALCL3
    J 6/63  ALH          J 6/70  ALO          J 9/64  ALOCL        J12/67  ALOH         J12/68  ALO2
    J12/68  ALO2H        J 6/70  AL2CL6       J 6/72  AL2O         J 9/65  AL2O2        J 6/72  AL2O3(S)
    J 6/72  AL2O3(L)     L 5/66  AR           J 3/61  C(S)         J12/69  CCL          J12/68  CCL2
    J 6/70  CCL3         J12/68  CCL4         J12/67  CH           J12/72  CH2          J 3/61  CH2O
    J 6/69  CH3          J 3/61  CH4          J 6/69  CN           J 6/66  CNN          J12/70  CN2
    J 9/65  CO           J12/65  COCL         J 6/61  COCL2        J 3/61  COS          J 9/65  CO2
    J12/62  CS           J 6/61  CS2          J12/69  C2           J12/68  C2CL2        J 3/67  C2H
    J 3/61  C2H2         J 9/65  C2H4         L 5/72  C2H6         J 3/67  C2N          J 3/61  C2N2
    J 9/66  C2O          J 6/68  C3O2         J 6/72  CL           J 6/66  CLCN         J 6/61  CLO
    J 3/61  CLO2         J 9/65  CL2          J12/65  CL2O         J 3/65  FE(S)        J 3/65  FE(S)
    J 3/65  FE(S)        J 3/65  FE(L)        J 3/65  FE           J 6/65  FECL         J12/70  FECL2(S)
    J12/70  FECL2(L)     J12/70  FECL2        J 6/65  FECL3(S)     J 6/65  FECL3(L)     J 6/65  FECL3
    J 6/65  FEO(S)       J 6/65  FEO(L)       J 9/66  FEO          J 6/66  FEO2H2(S)    J12/66  FEO2H2
    J 6/66  FEO3H3(S)    J12/70  FE2CL4       J 6/65  FE2O3(S)     J 6/65  FE3O4(S)     J 9/65  H
    J 3/64  HALO         J 9/64  HCL          L12/69  HCN          J12/70  HCO          J12/70  HNCO
    J 3/63  HNO          J 6/63  HNO2         J 6/63  HNO3         J 3/64  HO2          J 3/61  H2
    L11/65  H2O(L)       J 3/61  H2O          L 2/69  H2O2         J12/65  H2S          J 3/61  IC(S)
    J 3/61  N            J12/70  NCO          J12/71  NH           J12/65  NH2          J 9/65  NH3
    J 6/63  NO           J12/72  NOCL         J 9/64  NO2          J12/65  NO2CL        J12/64  NO3
    J 9/65  N2           J12/65  N2H4         J12/64  N2O          J 9/64  N2O4         J12/64  N2O5
    J12/70  N3           J 6/62  O            J12/70  OH           J 9/65  O2           J12/65  S(S)
    J12/65  S(L)         J 6/71  S            J 6/67  SH           J 6/61  SN           J 6/71  SO
    J 6/61  SO2          J 6/71  SO2CL2       J 9/65  SO3          J12/65  S2           J 9/67  SIO
    J 6/67  SIO2(S)      J 6/67  SIO2(S)      J 6/67  SIO2(S)      J 6/67  SIO2(L)      J 9/67  SIO2
    J12/71  SIS          J 3/67  SI2C

 READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
RIPS)
```

```
OF -      827273
                    OXIDIZER/COAL-    9100     WATER/COAL-    1000     CARBON CONVERSION-    9450

                         LOW TEMPERATURE THERMO EXTENSION IN CPHS AT TT -  298 150002 DEGREES KELVIN

                   FUEL             OXIDANT            MIXTURE

H  CAL/G      - 94422578+03       00000000         - 51674047+03

KG-ATOMS/KG
C               48142209-01       00000000           26346483-01

H               52995222-01       00000000           29002360-01

N               99234640-03       00000000           54307624-03

O               12785041-01       59377227-01        33879015-01

S               11624349-02       00000000           63615839-03

IC              28020050-02       00000000           15334356-02

CL              33340215-04       00000000           18245889-04

SI              12858276-02       00000000           70368676-03

FE              47009607-03       00000000           25726651-03

AL              57112435-03       00000000           31255561-03

AR              00000000          12516271-02        56665704-03

PT      C         H         N         O         S         IC        CL        SI         FE        AL        AR
          ADD AL2O3(S)
 1  -10 968  -10 377  -15 904  -24 093  -14 967   -2 659  -29 958  -15 915   -3 639  -14 322  -25 445   17 000
          ADD SIO2(S)
 1  -11 395  -10 436  -15 971  -22 518  -15 114   -2 744  -29 254  -16 363   -4 714  -25 443  -25 528    6 000
          PHASE CHANGE. REPLACE SIO2(S)      WITH SIO2(L)
 1  -12 046  -10 542  -16 100  -22 601  -15 427   -2 914  -28 917  -19 308   -6 741  -23 458  -25 686    5 000
          ADD FE(L)
 1  -12 035  -10 540  -16 098  -22 615  -15 421   -2 912  -28 921  -19 367   -6 714  -23 478  -25 684    2 000
 1  -12 151  -10 558  -16 116  -22 465  -15 483   -2 937  -28 866  -19 183   -8 080  -23 248  -25 705    4 000


READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
MIPS>
```

```
                              THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                                                PRESSURES
                                                                          WT FRACTION  ENTHALPY     STATE     TEMP      DENSITY
                                                                                        CAL/MOL               DEG  K     G/CM3
              CHEMICAL FORMULA                                                                                            0000
FUEL     C  49 7311    H  44 3187   N   1 0251   O   3 7243   S   1 2008    73034  -222076 750       S       298 15      0000
FUEL     IC  1 0000                                                         03366          000       S       298 15      0000
FUEL     CL  2 0000                                                         00118          000       G       298 15      0000
FUEL     SI  1 0000    O   2 0000                                           07726  -217699 047       S       298 15      0000
FUEL     FE  2 0000    O   3 0000                                           03754  -197250 043       S       298 15      0000
FUEL     AL  2 0000    O   3 0000                                           02912  -400493 262       S       298 15      0000
FUEL     H   2 0000    O   1 0000                                           09091   -57189 437       G       373 15      0000
OXIDNT   O   2 0000                                                         95000          000       G       298 15      0000
OXIDNT   AR  1 0000                                                         05000          000       G       298 15
             O/F=    8273    PERCENT FUEL= 54 7264    EQUIVALENCE RATIO=  2 1776    DENSITY=    0000
                 OXIDIZER/COAL=    9100    WATER/COAL=    100      CARBON CONVERSION=    9450

THERMODYNAMIC PROPERTIES

PRESS PSIA        15 000
TEMP DEG F      3447 10
ENTH BTU/LB     -930 13
S BTU/(LB-R)       2 6403
DENSITY L/F**3 8 492-03

M MOL WEIGHT      23 7175
(DLV/DLP) T       -1 0065
(DLV/DLT) P        1 1430
CP CAL/(G)(K)        7031
GAMMA (S)          1 1753
SON VEL M/SEC   1191 73




 READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
MIPS)
```

```
                 OXIDIZER/COAL=    9100     WATER/COAL=    1000     CARBON CONVERSION=    9450

 MOLE FRACTIONS

 ALO2H            7 679-07
 AL2O3(S)         3 501-03
 AR               1 270-02
 CO               5 495-01
 COS              4 342-04
 CO2              4 032-02
 CS               2 344-05
 CS2              1 022-06
 [illegible]      2 785-96
 FECL             3 811-03
 FE               1 876-03
 FECL2            9 580-07
 FEO              2 159-05
 FEO2H2           5 450-05
 H                2 188-03
 HCL              4 036-04
 H2               2 311-01
 H2O              8 658-02
 H2S              4 854-03
 IC(S)            3 436-02
 NO               8 163-07
 N2               6 083-03
 O                7 293-07
 OH               1 079-04
 S                4 359-04
 SH               1 895-03
 SO               8 704-04
 SO2              5 018-04
 S2               2 552-03
 SIO              1 995-03
 SIO2(L)          1 364-02
 SIO2             3 464-06
 SIS              1 323-24

 HHV COAL B/LB   12141 00
 MIXTURE MW         22 406
 MF OF CDG           83976
 V SAT SCF/LB   29 01858
 HHV SAT B/SCF     294 69
 EFFICIENCY          70435
 V DRY SCF/LB   28 58918
 HHV DRY B/SCF     299 12
 LHV SAT B/SCF     281 06
 LHV DRY B/SCF     285 28
 $ PER MMBTU         2 84


 READ COPY - THIS INPUT WILL NOT BE INTERPRETED
MIPS)
```

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5.0 SAMPLE PROBLEM 2

The following pages which could be a continuation of Sample 1, indicate the procedures to be used to edit existing coal data and/or existing namelist data.

The data set, after editing will still be the same as in the attached memo, but additional namelist options are illustrated.

```
TYPE  YES  FOR PRINT TO PRINT FILE
RIPS> NO
```

```
LEWIS CHEMICAL EQUILIBRIUM PROGRAM

          MAIN MENU

 1 - INSERT THERMODYNAMICS DATA
 2 - INSERT LOW TEMP EXTENSION THERMO DATA
 3 - INSERT OR EDIT REACTANTS
 4 - OMIT SPECIES FROM THERMO DATA
 5 - INSERT CONDENSED SPECIES
 6 - INSERT OR EDIT NAMELIST
 7 - START PROGRAM CALCULATION
 8 - INSERT OR EDIT COAL DATA
 RETURN - TERMINATE PROGRAM
MIPS>8
```

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```
 TYPE YES TO READ IN PREVIOUS COMPOSITION
MIPS>YES
```

```
 TYPE YES TO READ IN PREVIOUS COMPOSITION
RIPS) ES
 1 - VOLATILE (OPTIONAL) AND ASH AS LBS/100 LBS DRY COAL
      VOLATILE    37 5400
      ASH         19 8300

 2 - COAL TEMPERATURE IN DEG F      77 00

 3 - DRY COAL COMPOSITION AS LBS/100 LBS DRY COAL
     C            67 3100
     H             4 7570
     N             1 5290
     O             6 3430
     S             4 1000

 4 - OTHER COAL COMPONENTS AS LBS/100 LBS DRY COAL. STATE AND COMPOSITION
      1300          G     CL    2 0000             0000          0000          0000          0000

 5 - ASH COMPOSITION AS LBS/100 LBS ASH AND COMPONENT
   53 6800                SI    1 0000  0     2 0000             0000          0000          0000
   26 0800                FE    2 0000  0     3 0000             0000          0000          0000
   20 2300                AL    2 0000  0     3 0000             0000          0000          0000

 6 - FRACTION CARBON CONVERSION       9450

 7 - HEATING VALUE OF COAL BTU/LB    12141 000

 8 - OTHER FUEL COMPONENTS AS LBS/LB COAL. TEMPERATURE IN DEG F. STATE AND COMPOSITION
      1000   212 000 G    H     2 0000  0     1 0000             0000          0000          0000

 9 - OXIDIZER TEMPERATURE IN DEG F      77 00

 10 - OXIDIZER COMPONENTS AS LBS/100 LBS OXIDIZER AND COMPONENT
   95 0000                O     2 0000             0000          0000          0000          0000
    5 0000                AR    1 0000             0000          0000          0000          0000

 TYPE 1 OR 2 TO MODIFY OR REPLACE
     RETURN TO CONTINUE
RIPS)1
 TYPE GROUP NUMBERS OF DATA TO BE CHANGED IN ASCENDING ORDER    FOR EXAMPLE 1 3 7 9
RIPS)2 5 6
```

```
 TYPE COAL TEMPERATURE IN DEG F
MIPS>77
 GROUP NUMBER     5
   1    53 6800                   SI     1 0000  0      2 0000          0000          0000          0000
   2    26 0800                   FE     2 0000  0      3 0000          0000          0000          0000
   3    20 2300                   AL     2 0000  0      3 0000          0000          0000          0000
 TYPE 1-ALTER. 2-DELETE  3-ADD. RETURN TO CONTINUE
MIPS>1
 TYPE LINE NUMBER
MIPS>1
 LBS/100 LBS DRY ASH AND COMPONENT
MIPS>53 68 2HSI 1  1HO 2
   1    53 6800                   SI     1 0000  0      2 0000          0000          0000          0000
   2    26 0800                   FE     2 0000  0      3 0000          0000          0000          0000
   3    20 2300                   AL     2 0000  0      3 0000          0000          0000          0000
 TYPE 1-ALTER. 2-DELETE  3-ADD. RETURN TO CONTINUE
MIPS>
 TYPE CARBON CONVERSION FRACTION. FOR EXAMPLE. 0 89
MIPS>0 945
```

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```
INDEX                          REACTANT(*)                                 REL WT/   MOLE  ENTHALPY/    PHASE  TEMP.K   FUEL/  DENSITY
                                                                           NO MOLES        INT ENERGY                   OXID
 1  C   49 7311  H  44 3187  N   1 0251  0   3 7243  S   1 2008   730336    -222076 6875    S    298 150    F      00000
 2  IC   1 0000        0000        0000        0000        0000   033655          0000*    S    298 150    F      00000
 3  CL   2 0000        0000        0000        0000        0000   001182          0000*    G    298 150    F      00000
 4  SI   1 0000  0   2 0000        0000        0000        0000   077258          0000*    S    298 150    F      00000
 5  FE   2 0000  0   3 0000        0000        0000        0000   037535          0000*    S    298 150    F      00000
 6  AL   2 0000  0   3 0000        0000        0000        0000   029116          0000*    S    298 150    F      00000
 7  H    2 0000  0   1 0000        0000        0000        0000   090909          0000*    G    373 150    F      00000
 8  O    2 0000        0000        0000        0000        0000   950000          0000*    G    298 150    O      00000
 9  AR   1 0000        0000        0000        0000        0000   050000          0000*    G    298 150    O      00000
                                                    *     INDICATES ENTHALPY TO BE CALCULATED

 TYPE  1. 2.OR 3  TO MODIFY. DELETE. OR ADD A REACTANT (RETURN TO CONTINUE)
MIPS>
TYPE YES FOR SPECIAL OMITS FOR COAL DATA
MIPS>YES
```

```
LEWIS CHEMICAL EQUILIBRIUM PROGRAM

          MAIN MENU

 1 - INSERT THERMODYNAMICS DATA
 2 - INSERT LOW TEMP EXTENSION THERMO DATA
 3 - INSERT OR EDIT REACTANTS
 4 - OMIT SPECIES FROM THERMO DATA
 5 - INSERT CONDENSED SPECIES
 6 - INSERT OR EDIT NAMELIST
 7 - START PROGRAM CALCULATION
 8 - INSERT OR EDIT COAL DATA
 RETURN - TERMINATE PROGRAM
MIPS>6
```

```
TYPE YES FOR PRINT INPT2 NAMELIST
MIPS>YES
 $INPT2
 DETN    =  F
 ERATIO  =  F
 FA      =  F
 FPCT    =  F
 HP      =  T
 IDEBUG  =             +0
 IONS    =  F
 MIX     =       91000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00
 MMHG    =  F
 NSOM    =  F
 OF      =  T
 P       =       15000000E+02,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00
 PSIA    =  T
 RKT     =  F
 S0      =       00000000E+00
 SHOCK   =  F
 SO      =       00000000E+00
 SP      =  F
 SU      =  F
 T       =       00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00
 TP      =  F
 TU      =  F
 UU      =  F
 U       =       00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00,     00000000E+00,     00000000E+00,     00000000E+00,
                 00000000E+00

 $END
 BEGIN NAMELIST INPT2 INPUT
> $INPT2 HP= F , T=2500 , TP= T  $END
```

ORIGINAL PAGE IS
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```
$IMPT2
DETN     =  F
ERATIO   =  F
FA       =  F
FPCT     =  F
HP       =  F
IDEBUG   =             +0
IONS     =  F
MIX      =
              91000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00
MMHG     =  F
NSQM     =  F
OF       =  T
P        =
              15000000E+02,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00
PSIA     =  T
RKT      =  F
S0       =
              00000000E+00
SHOCK    =  F
SO       =
              00000000E+00
SP       =  F
SU       =  F
T        =
              25000000E+04,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00
TP       =  T
TV       =  F
UV       =  F
V        =
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
              00000000E+00

$END




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MIPS>
```

```
LEWIS CHEMICAL EQUILIBRIUM PROGRAM

          MAIN MENU

 1 - INSERT THERMODYNAMICS DATA
 2 - INSERT LOW TEMP EXTENSION THERMO DATA
 3 - INSERT OR EDIT REACTANTS
 4 - OMIT SPECIES FROM THERMO DATA
 5 - INSERT CONDENSED SPECIES
 6 - INSERT OR EDIT NAMELIST
 7 - START PROGRAM CALCULATION
 8 - INSERT OR EDIT COAL DATA
 RETURN - TERMINATE PROGRAM
MIPS>7
```

```
SPECIES BEING CONSIDERED IN THIS SYSTEM
   J12/65  AL          J 6/70  ALCL        J 6/70  ALCL3(S)    J 6/70  ALCL3(L)    J 6/70  ALCL3
   J 6/63  ALH         J 6/70  ALO         J 9/64  ALOCL       J12/67  ALOH        J12/68  ALO2
   J12/68  ALO2H       J 6/70  AL2CL6      J 6/72  AL2O        J 9/65  AL2O2       J 6/72  AL2O3(S)
   J 6/72  AL2O3(L)    L 5/66  AR          J 3/61  C(S)        J12/69  CCL         J12/68  CCL2
   J 6/70  CCL3        J12/68  CCL4        J12/67  CH          J12/72  CH2         J 3/61  CH2O
   J 6/69  CH3         J 3/61  CH4         J 6/69  CN          J 6/66  CNN         J12/70  CN2
   J 9 65  CO          J12/65  COCL        J 6/61  COCL2       J 3/61  COS         J 9/65  CO2
   J12/62  CS          J 6/61  CS2         J12/69  C2          J12/68  C2CL2       J 3/67  C2H
   J 3/61  C2H2        J 9/65  C2H4        L 5/72  C2H6        J 3/67  C2N         J 3/61  C2N2
   J 9/66  C2O         J 6/68  C3O2        J 6/72  CL          J 6/66  CLCN        J 6/61  CLO
   J 3/61  CLO2        J 9/65  CL2         J12/65  CL2O        J 3/65  FE(S)       J 3/65  FE(S)
   J 3/65  FE(S)       J 3/65  FE(L)       J 3/65  FE          J 6/65  FECL        J12/70  FECL2(S)
   J12/70  FECL2(L)    J12/70  FECL2       J 6/65  FECL3(S)    J 6/65  FECL3(L)    J 6/65  FECL3
   J 6/65  FEO(S)      J 6/65  FEO(L)      J 9/66  FEO         J 6/66  FEO2H2(S)   J12/66  FEO2H2
   J 6/66  FEO3H3(S)   J12/70  FE2CL4      J 6/65  FE2O3(S)    J 6/65  FE3O4(S)    J 9/65  H
   J 3/64  HALO        J 9/64  HCL         L12/69  HCN         J12/70  HCO         J12/70  HNCO
   J 3/63  HNO         J 6/63  HNO2        J 6/63  HNO3        J 3/64  HO2         J 3/61  H2
   L11/65  H2O(L)      J 3/61  H2O         L 2/69  H2O2        J12/65  H2S         J 3/61  IC(S)
   J 3/61  N           J12/70  NCO         J12/71  NH          J12/65  NH2         J 9/65  NH3
   J 6/63  NO          J12/72  NOCL        J 9/64  NO2         J12/65  NO2CL       J12/64  NO3
   J 9/65  N2          J12/65  N2H4        J12/64  N2O         J 9/64  N2O4        J12/64  N2O5
   J12/70  N3          J 6/62  O           J12/70  OH          J 9/65  O2          J12/65  S(S)
   J12/65  S(L)        J 6/71  S           J 6/67  SH          J 6/61  SN          J 6/71  SO
   J 6/61  SO2         J 6/71  SO2CL2      J 9/65  SO3         J12/65  S2          J 9/67  SIO
   J 6/67  SIO2(S)     J 6/67  SIO2(S)     J 6/67  SIO2(S)     J 6/67  SIO2(L)     J 9/67  SIO2
   J12/71  SIS         J 3/67  SI2C



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RIPS)
```

```
OF •      827273
                    OXIDIZER/COAL•    9100     WATER/COAL•    1000     CARBON CONVERSION•    9450
                     FUEL               OXIDANT              MIXTURE

H  CAL/G        - 94422572+03         00000000           - 51674044+03

KG-ATOMS/KG
C                 48142209-01         00000000             26346483-01

H                 52995222-01         00000000             29002360-01

N                 99234840-03         00000000             54307624-03

O                 12785041-01         59377227-01          33879015-01

S                 11624349-02         00000000             63615839-03

IC                28020050-02         00000000             15334356-02

CL                33340215-04         00000000             18245889-04

SI                12858276-02         00000000             70368676-03

FE                47009607-03         00000000             25726651-03

AL                57112435-03         00000000             31255561-03

AR                00000000            12516271-02          56665704-03

PT       C         H        N         O         S          IC        CL        SI         FE        AL        AR
            ADD AL2O3(S)
 1     -9 188   -10 135  -15 662   -26 504   -14 718    -2 362   -31 193   -14 064       13   -13 333   -25 133   17 000
            ADD FE3O4(S)
 1     -9 171   -10 127  -15 660   -26 516   -14 728    -2 362   -30 929   -14 048       137  -30 310   -25 130    5 000
            ADD SIO2(S)
 1     -9 151   -10 119  -15 659   -26 532   -14 739    -2 362   -30 060   -14 031    -4 764  -30 286   -25 127    5 000
            ADD FE(S)
 1     -8 950   -10 094  -15 650   -26 702   -14 574    -2 362   -30 074   -24 839    -4 538  -30 032   -25 111    5 000
 1    -10 979   -10 439  -15 651   -24 994   -14 115    -2 362   -29 706   -28 254    -6 814  -32 593   -25 112    5 000
 1     -9 032   -10 102  -15 650   -26 627   -14 561    -2 362   -30 038   -24 989    -6 814  -30 144   -25 111    5 000




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MIPS>
```

SAVE

EQLBRM

```
                                        THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                                                     TEMPERATURE AND PRESSURE

                                                                                      WT FRACTION  ENTHALPY    STATE   TEMP    DENSITY
           CHEMICAL FORMULA                                                                        CAL/MOL             DEG  K   G/CM3
FUEL     C  49 7311   H  44 3187   N   1 0251   O   3 7243   S   1 2008        73034  -222076 687     S    298 15    0000
FUEL     IC  1 0000                                                            03366             000     S    298 15    0000
FUEL     CL  2 0000                                                            00118             000     G    298 15    0000
FUEL     SI  1 0000    O   2 0000                                              07726  -217699 047     S    298 15    0000
FUEL     FE  2 0000    O   3 0000                                              03754  -197250 043     S    298 15    0000
FUEL     AL  2 0000    O   3 0000                                              02912  -400453 262     S    298 15    0000
FUEL     H   2 0000    O   1 0000                                              09091   -57189 437     G    373 15    0000
OXIDNT   O   2 0000                                                            95000             000     G    298 15    0000
OXIDNT   AR  1 0000                                                            05000             000     G    298 15    0000

              O/F=    8273    PERCENT FUEL= 54 7264    EQUIVALENCE RATIO=  2 1776    DENSITY=     0000
                 OXIDIZER/COAL=    9100     WATER/COAL=    1000    CARBON CONVERSION=    9450

THERMODYNAMIC PROPERTIES


PRESS PSIA        15 000
TEMP DEG F      2500 00
ENTH BTU/LB    -1394 67
S BTU/(LB-R)      2 5055
DENSITY L/F**3 1 133-02

M MOL WEIGHT     23 9647
(DLV/DLP) T      -1 0006
(DLV/DLT) P       1 0092
CP CAL/(G)(K)       4231
GAMMA (S)         1 2485
SON VEL M/SEC   1040 62




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MIPS>
```

OUT1

OUT2

```
                 OXIDIZER/COAL=    9100     WATER/COAL=    1000     CARBON CONVERSION=    9450

MOLE FRACTIONS

AL2O3(S)         3 521-03
AR               1 277-02
CO               5 397-01
COS              9 251-04
CO2              5 301-02
CS               8 364-06
CS2              3 615-06
FE(S)            5 792-03
FE               2 150-06
FECL2            6 799-07
FEO2H2           2 680-06
H                4 014-05
HCL              4 097-04
H2               2 400-01
H2O              7 442-02
H2S              1 197-02
IC(S)            3 455-02
N2               6 118-03
OH               5 401-07
S                4 332-06
SH               2 246-04
SO               1 140-05
SO2              1 319-05
S2               5 828-04
SIO2(S)          1 586-02

HHV COAL B/LB   12141 60
MIXTURE MW         22 533
MF OF CDG           85165
V SAT SCF/LB    29 26287
HHV SAT B/SCF     290 28
EFFICIENCY          69964
V DRY SCF/LB    28 82986
HHV DRY B/SCF     294 64
LHV SAT B/SCF     276 32
LHV DRY B/SCF     280 47
$ PER MMBTU         2 86




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MIPS>
```

OUT3

OUT4

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```
LEWIS CHEMICAL EQUILIBRIUM PROGRAM

          MAIN MENU

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 7 - START PROGRAM CALCULATION
 8 - INSERT OR EDIT COAL DATA
 RETURN - TERMINATE PROGRAM
MIPS>
 . . . . . . . . . . . MIPS MODULE TERMINATED.  SUP'S USED .     26 SECONDS . . . . . . . . . . . .

NORMAL EXIT    CPU TIME        12388      TOTAL SUPS        27808    (MILLISECONDS)
-00COMPLETE
```

```
 TOTAL SUP TIME =   2.80 MIN
 IS THE CURRENT PRINT FILE TO BE TRANSMITTED?
MIPS>NO
 INSERT COMMANDS   (INSERT    HELP    FOR TUTORING)
MIPS>SP
  MIPS IS EXITING
 PRINT FILES WILL BE DELETED IF NOT TRANSMITTED
 IS THE CURRENT PRINT FILE TO BE TRANSMITTED?
MIPS>NO
NORMAL EXIT    CPU TIME:           20      TOTAL SUPS          7084    (MILLISECON
DS)STOP  MIPS
>@FIN



  PUNID  LEWIST   ACCT: 1HPD013K0000   PROJECT: SEVIGNBIN208
       LOAD BLANK TP6 N25LEWIS -1 LEWIST
      ***   SAVE  ***   24609 TP6   N25LEWIS
   SEVIGNBIN208*N25LEWIS       24609        082180
       STOP  MIPS
      LEWIST FIN
  TIME      TOTAL  00:02:52.840      CBSUPS:  047260104
            CPU    00:00:10.552      I/O   00:01:24.660
            CC/ER  00:01:17.627      WAIT: 00:27:40.234
  IMAGES  READ     116       PAGES    13
  START     10:39:03 AUG 18,1980    FIN   11:12:02 AUG 18,1980

********************************************************************************
* THERE WILL BE A USERS MEETING ON 9/10/80 AT 09:00 A.M  IN THE HOSC           *
* CONFERENCE ROOM AT BLDG. 4663  ALL USERS ARE URGED TO ATTEND.                *
********************************************************************************
------------------------------------------------------------------------
DEMAND USERS   PLEASE KEYIN  @USER*RESPONSE.POLL   PRIOR TO @FIN  ( THANK YOU)
------------------------------------------------------------------------
*TERMINAL INACTIVE*
>
```

APPENDIX A

APPLICATION OF LEWIS CHEMICAL EQUILIBRIUM COMPUTER PROGRAM TO COAL GASIFICATION

BY

DAVID SEYMOUR

This copy of a NASA memo describes the calculations of input and output used in the sample problems for conversion to coal gasification data.

National Aeronautics and
Space Administration

George C. Marshall Space Flight Center
Marshall Space Flight Center, Alabama
35812

NASA

Reply to Attn of: PF15 E(80-118)

August 28, 1980

TO: PF15/John P. McCarty

FROM: PF15/David C. Seymour

SUBJECT: Application of the Lewis Chemical Equilibrium Computer Program to Coal Gasification

REF: (a) "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations" NASA SP-273, Gordon and McBride

(b) "Fortran IV Computer Program for Calculation of Thermodynamic and Transport Properties of Complex Chemical Systems", NASA TN-D-7056, Svehla, McBride

In the early 1960's Lewis Research Center developed a chemical equilibrium combustion (CEC) computer program for rocket engine performance analysis (Ref. (a)). Because of the thorough documentation, flexibility, and comprehensive specie library, the program has become an aerospace industry standard.

The CEC program can be applied to entrained flow coal gasification without modification. The complete thermodynamic state can be described for either adiabatic combustion or specified temperature and pressure. The procedures used to apply the program to coal gasification are described here, together with a sample case. Because these procedures are somewhat tedious and error prone, a subroutine has been added to the CEC program which contains these procedures.

The CEC program requires the chemical formula, relative amount and enthalpy of each reactant in the system. For a typical entrained flow gasifier, the reactants include steam, oxygen (with nitrogen and argon impurities) and coal. Due to the complex composition of coal, the chemical formulae for the coal components are generally not supplied and must be determined from an elemental analysis.

Consider the ultimate analysis of the dry Kentucky #9 used by TVA for design criteria.

Coal Composition

Element	% Wt.
C	67.31
H	4.757
N	1.529
O	6.343
S (Pyritic)	2.517
S (Non Pyritic)	1.583
Cl	.131
Ash	15.83
	100.00

Ash Composition

Compound	% Wt.
S_iO_2	45.94
Al_2O_3	17.31
$F_{e2}O_3$	22.29
C_aO	5.486
M_gO	1.164
SO_3	3.264
$N_{a2}O$	.557
K_2O	2.336
T_iO_2	.742
Other	.911
	100.00

The term ash used here refers to the residue obtained from complete oxidation of the coal with excess air during a proximate analysis of the coal.

The compounds existing in the coal are unknown. In particular, the composition of the ash is not the same as the composition of the minerals in the coal and thus the ash mass fraction in the coal indicated above is not the true mineral content of the coal. The sodium and potassium, for example, probably exist in the coal as chlorine salts or as part of the other inorganic compounds. Most of the iron in the coal exists as iron pyrite, F_eS_2.

The details of the compounds in the coal and ash are not required for an equilibrium combustion calculation. Only the relative amounts of the elements present must be known. The ash composition shown above is actually an elemental composition with ficticious oxide compounds assumed and is not a real ash composition. The actual ash composition is dependant on the amount of oxygen available during combustion, the combustion temperature, and the rate of cooling of the combustion products.

The ultimate analysis of coal shown above consists of direct measurement of the amount of elemental C, H, N, S, and Cl. The ash weight is then added and the oxygen content is taken to be the difference between 100 and this sum. Thus, if the only remaining element in the coal is oxygen, the oxygen content which is obtained plus the oxygen in the ficticious ash compounds represents the true total elemental oxygen in the coal. The ficticious ash compounds can be used directly to describe the relative amounts of the elements and corrections to the ash content or further assumptions about the coal composition are not required The only exception is that the sulfur in the ash should not be included, since it is already accounted for in the elemental sulfur in the coal. However this correction is smaller than the accuracy of the data and is not included here.

Determination of CEC Reactant Data From Coal Composition

The elemental mass composition of the coal must be converted into a atom/(mole reactant) form for input to the CEC. Since the program is limited to five elements per reactant, a reacting coal is arbitrarily defined to be composed of C, H, N, O and S. Other elements and compounds known to exist in the coal are treated as individual reactants.

Since some of the carbon in the coal may not actually be oxidized, a carbon conversion factor, f, is defined as the mass fraction of carbon which participates in the reaction. The remaining carbon is removed from the reacting coal and treated as in inert solid with carbon thermodynamic properties.

As an example of the procedure, the composition of the reacting coal for the previously described Kentucky #9 is, with f = .945

Coal Element	lb Element / 100 lb coal	lb Element / 100 lb coal	lb Element / 100 lb reacting coal
C	67.31	63.61	79.18
H	4.757	4.757	5.921
N	1.529	1.529	1.903
O	6.343	6.343	7.896
S	4.10	4.10	5.103
Cl	.131	80.337	100.00
Ash	15.83		
	100.00		

Converting to lb-atoms/(lb-mole reacting coal) gives

Element	lb Element / lb-atom	lb-atoms / 100 lb reacting coal	lb-atoms / 100 lb-mole reacting coal
C	12.01	6.593	49.74
H	1.008	5.874	44.31
N	14.007	.136	1.03
O	16.00	.494	3.73
S	32.064	.159	1.20
		13.256	100.00

Then the chemical formula for the reacting coal is

$C_{49.74} H_{44.31} N_{1.03} O_{3.73} S_{1.20}$

and it's molecular weight per 100 lb-mole is

$\left(\frac{100}{13.256}\right) 100 = 754.4$ lb/(100 lb-mole)

= 754.4 g/(100 g-mole reacting coal)

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Relative Reactant Weights

In coal gasification it is convenient to use as independent variables the mass ratios water/coal (or steam/coal) and oxygen/coal. The CEC program, however, allows only one independent variable, oxidizer/fuel (O/F). The components of the system identified as oxidyzers as opposed to fuels is completely arbitrary. The distinction between oxidyzer and fuel is only important when running multiple O/F values within a single execution of the program.

The convention selected here is $\text{fuel} = \text{coal} + H_2O + (\text{other fuel compounds})$,

where $\text{coal} = \text{reacting coal} + \text{minerals} + \text{inert C} + (\text{other coal compounds})$.

$\text{Oxidyzer} = O_2 + (\text{impurities in } O_2 \text{ feed})$,

where the other fuel and coal compounds and the O_2 impurities must be included in the CEC thermodynamic data library.

Then

$$\frac{\text{coal}}{\text{fuel}} = \frac{1}{1 + \frac{H_2O}{\text{coal}} + \left(\frac{\text{other fuel compounds}}{\text{coal}}\right)}$$

and the relative weight of reacting coal in the fuel, required for input to the CEC is

$$\frac{\text{reacting coal}}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} \left(\frac{\text{reacting coal}}{\text{coal}}\right)$$

similarly, for the other components of the fuel,

$$\frac{\text{minerals}}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} \left(\frac{\text{minerals}}{\text{coal}}\right)$$

$$\frac{\text{inert C}}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} (1-f) \left(\frac{\text{carbon}}{\text{coal}}\right)$$

$$\frac{H_2O}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} \left(\frac{H_2O}{\text{coal}}\right)$$

and for the oxidyzer

$$\text{CEC O/F} = \frac{\text{coal}}{\text{fuel}} \left(\frac{O_2}{\text{coal}}\right)$$

where O_2/coal includes the impurities.

As an example, suppose an equilibrium calculation were to be run for Kentucky # 9 with $f = .945$, $H_2O/\text{coal} = .10$, and $O_2/\text{coal} = .91$, where the O_2 feed is 95% pure O_2 and 5% Ar by volume. Then the relative weights are

$$\frac{\text{coal}}{\text{fuel}} = \frac{1}{1 + .10} = .9091$$

$$\frac{\text{reacting coal}}{\text{fuel}} = .9091\ (.8034) = .7304$$

$$\frac{\text{minerals}}{\text{fuel}} = .9091\ (.1583) = .1439$$

$$\frac{\text{inert C}}{\text{fuel}} = .9091\ (1- .945)\ (.6731) = .0337$$

$$\frac{H_2O}{\text{fuel}} = .9091\ (.10) = .0909$$

$$\frac{Cl_2}{\text{fuel}} = .9091\ (.00131) = \underline{.0012}$$

$$1.000$$

$$\frac{O_2}{\text{Oxidyzer}} = .975$$

$$\frac{Ar}{\text{oxidyzer}} = .025$$

CEC O/F = .9091 (.91) = .8273

The relative weights of the ash components are, considering only the largest three,

$$\frac{S_iO_2}{\text{fuel}} = .1439\ \left(\frac{.4594}{.8554}\right) = .0773$$

$$\frac{Al_2O_3}{\text{fuel}} = .1439\ \left(\frac{.1731}{.8554}\right) = .0291$$

$$\frac{Fe_2O_3}{\text{fuel}} = .1439\ \left(\frac{.2229}{.8554}\right) = \underline{.0375}$$

$$.1439$$

where the remaining ash components have been arbitrarily spread equally between these three.

Determination of Coal Enthalpy from HHV

The CEC program requires an enthalpy for each reactant when calculating adiabatic flame conditions. Enthalpies are not required for calculating equilibrium conditions at specified temperature and pressure. The enthalpy of the reacting coal is the heat of formation at 25°C plus the enthalpy changes from 25°C to the coal temperature. HHV is the heat of combustion at 25°C, where the products of combustion are CO_2, H_2O (l), and SO_2. The HHV of coal is either measured in a calorimeter bomb test or obtained from an empirical formula based on the coal ultimate analysis.

The known HHV_{coal} can be broken down into the reacting components selected for CEC input as

$$HHV_{coal} = HHV_{r.c.} \frac{(\text{reacting coal})}{\text{coal}} + HHV_c \frac{(\text{inert C})}{\text{coal}}$$

The oxides in the ash all have an HHV of zero and do not have to be included here.

The HHV for carbon can be calculated from the heats of formation and the definition of HHV. For carbon,

$$C + O_2 \xrightarrow{25^oC} CO_2$$

$$HHV_c = (\Delta h_f C + \overset{o}{\cancel{\Delta b_f O_2}}) - (\Delta h_f CO_2)$$

Where $\Delta h_f C$ = heat of formation of carbon, taken here to be amorphous carbon. $\Delta h_f C$ = 4680 BTU/lb-mole
Δh_{CO_2} = -169293 BTU/lb-mole

$$HHV_c = (4680 + 169293) \frac{1}{12.01} = 14486 \text{ BTU/lb carbon}$$

Then the reacting coal HHV is

$$HHV_{rc} = \frac{HHV_{coal} - 14486 \frac{(\text{inert C})}{\text{coal}}}{\frac{\text{reacting coal}}{\text{coal}}}$$

if, in the previous example, HHV_{coal} is given as 12141 BTU/lb coal then

$$HHV_{rc} = \frac{12141 - 14486\ (.037)}{.8034}$$

$$= \frac{12141 - 536}{.8034}$$

$$= 14445 \text{ BTU/lb reacting coal}$$

The heat of formation of the reacting coal can be obtained from the definition of HHV. The reaction is

$$\text{reacting coal} + \text{excess } O_2 \longrightarrow X_c CO_2 + \frac{X_h}{2} H_2O\,(l) + X_s\, SO_2$$

where X_c, H_h, X_s are the C, H, and S g-atoms per 100 g-moles of reacting coal.

The N and O in the coal are not included since their heat of formation is zero.

Then $$HHV_{rc} = \Delta h_{f_{rc}} - (X_c \Delta h_{fCO_2} + \frac{X_h}{2} \Delta h_{fH_2O} + X_s \Delta h_{fSO_2})$$

where $\Delta h_{fCO_2} = -94051.8$ cal/g-mole CO_2

$\Delta h_{fH_2O}\,(l) = -68317.4$ cal/g-mole $H_2O\,(l)$

$\Delta h_{fSO_2} = -70960$ cal/g-mole SO_2

$$\Delta h_{f_{rc}} = HHV_{rc} - X_c\,(94051.8) - X_h\,(68317.4) - X_s\,(70960)$$

where the units of $\Delta h_{f_{rc}}$ required by the CEC are cal/(100 g-mole reacting coal).

In the previous example,

$$HHV_{rc} = \left(14445 \frac{\text{BTU}}{\text{lb reacting coal}}\right)\left(\frac{\text{cal/g}}{1.8\ \text{BTU/lb}}\right)\left(754.4 \frac{\text{g}}{100\ \text{g-mole}}\right)$$

$$= 6.0540 \times 10^6\ \text{cal/(100 g-mole)}$$

and

$$\Delta h_{f_{rc}} = 6.0540 \times 10^6 - (49.74)\,(94051.8) - \frac{(44.31)}{2}\,(68317.4) - (1.20)\,(70960)$$

$$= 6.0540 \times 10^6 - 6.2769 \times 10^6$$

$$= -222890\ \text{cal/(100 g-mole reacting coal)}$$

If the coal temperature were 25°C (77°F), then the coal enthalpy required by the CEC would be $\Delta h_{f_{rc}}$. For temperatures up to about 200°F, the reacting coal enthalpy can be estimated from the emperical equation.

$$h_{rc} - \Delta h_{f_{rc}} = .175\,(T - 77) + .0029 W_v\,(T - 77) + .00025\,(T - 60)^2 - .072$$

where T is the coal temperature in °F and W_v is the percent of volitiles in the dry, ash free coal given by proximate analysis.

If in the previous example, the proximate analysis were

Volitiles	37.54	37.54	44.60
Fixed Carbon	46.63	46.63	55.40
Ash	15.83	84.17	100.00
	100.00		

then W_v = 44.60 and if the coal temperature were 100°F

$$h_{rc} - \Delta h_{f_{rc}} = .175\,(23) + .0029\,(44.6)\,(23) = .00025\,(40)^2 - .072$$

$$= 7.33\ \frac{\text{BTU}}{\text{lb reacting coal}}$$

$$= (7.33)\ \frac{754.4}{1.8} = 3072\ \text{cal/(100 g-mole reacting coal}$$

and the enthalpy used in the CEC, h_{rc}, would be

$$h_{rc} = -222890 + 3072 = -219820\ \text{cal/(100 g-mole)}$$

The enthalpy of the remaining reactants will automatically be determined by the CEC program from a specified reactant temperature.

Use and Interpretation of CEC Results

The CEC output consists of the thermodynamic state variables and the specie mole fractions. For coal gasification several other parameters are of interest.

First, the molecular weight output by the program is an effective value meant for use in the ideal gas equation of state. This effective value is the mass of the system per mole of gas in the system and excludes the moles of solids and liquids. To convert to a true ratio of mass/mole for the system,

$$M_w = (\text{CEC } M_w)\,(1 - \sum_{\substack{\text{solid}\\+\\\text{liquids}}} X_i)$$

where X_i = CEC mole fraction.

Historically, fuel gas properties are usually quoted on a standard cubic foot basis, with various conventions taken for standard conditions. The standard used here is a saturated gas at 60°F and 30 in. of mercury. With this standard 385.2 SCF will contain 1 lb-mole of dry fuel gas. If the standard were dry gas at 60°F and 30 in. of mercury, 379.5 SCF would contain 1 lb-mole of dry fuel gas.

The moles of dry product gas per total moles of reactants is taken to be

$$X_{DP} = X_{CO} + X_{H2} + X_{CH4} + X_{CO2} + X_{N2} + X_{Ar}$$

The volume of clean, dry gas produced per lb of coal is then

$$Y_{DP} = \frac{385.2\, X_{DP}}{M_w} \frac{\text{Reactants}}{\text{coal}}, \text{ SCF/(lb coal)}$$

where the mass fraction $\left(\frac{\text{Reactants}}{\text{coal}}\right)$ can be obtained as $\left(\frac{\text{fuel}}{\text{coal}} + \frac{O_2}{\text{coal}}\right)$.

The higher heating value of the gas, in BTU/SCF, is obtained from the HHV of the constituents as

$$HHV = \frac{319.24\, X_{H2} + 316.06\, X_{CO} + 994.4\, X_{CH4}}{X_{DP}}$$

The lower heating value, which takes water vapor rather than liquid water as the reference state, is given by

$$LHV = \frac{269.71\, X_{H2} + 316.06\, X_{CO} + 895.3\, X_{CH4}}{X_{DP}}$$

Cold gas efficiency, which is the fraction of the coal chemical energy converted to a gas chemical energy, is

$$E = \frac{HHV\, Y_{DP}}{HHV\ \text{coal}}$$

where HHV $_{\text{coal}}$ is the higher heating value of dry coal and does not include any of the previously discussed corrections for carbon conversion.

The equilibrium thermochemical data provided by the program represent an idealized state and must be applied to actual gasifier operation with caution. The major non-equilibrium effect, unreacted carbon, had been accounted for in this application of the CEC program. However, as the gas/particle mixture is cooled within the gasifier, the chemical reaction rates will decrease and chemical equilibrium will no longer be maintained. A freeze point emperature can be defined as that temperature at which the equilibrium composition approximates the final non-equilibrium temperature. This freeze point temperature must be determined by a finite rate analysis or experimental data. When the freeze point temperature is known, the CEC program can be applied with a specified temperature and pressure to describe the final gas composition.

If transport property data is required, the CEC program described in Ref (B) can be used in lieu of Ref. (A).

David C. Seymour

Distribution:
PF15/Messrs. Rutland/Klan/Irby/Costes/Deaton/Garrett/Hyde/Johnston/
  Kramer/Larsen/Lynn/Middleton/Stonemetz
PF15/Dr. Proffitt
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PD33/Mr. Stafford
PD31/Messrs. Cole/Goss/Steincamp/Wheeler/Belcher
PP03/Mr. Hamaker
EF43/Messrs. Piner/Spear

APPENDIX B

SOURCE LISTING OF PROGRAM ELEMENTS WITH MODIFICATIONS

This is a printout of the Lewis Chemical Equilibrium Program with the modifications necessary for coal gasification data.

```
LL              EEEEEEEEEEEE    WW        WW       IIIIII        SSSSSSSS      TTTTTTTTTTTT
LL              EEEEEEEEEEEE    WW        WW       IIIIII       SSSSSSSSSS     TTTTTTTTTTTT
LL              EE              WW        WW         II        SS        SS         TT
LL              EE              WW        WW         II        SSS       SS         TT
LL              EE              WW        WW         II         SSS                 TT
LL              EEEEEEEE        WW   WW   WW         II           SSS               TT
LL              EEEEEEEE        WW  WWWW  WW         II             SSS             TT
LL              EE              WW WWWWWW WW         II               SSS           TT
LL              EE              WWWWW  WWWWW         II        SS        SS         TT
LL              EE              WWWW    WWWW         II        SS        SS         TT
LLLLLLLLLLLL    EEEEEEEEEEEE    WWW      WWW       IIIIII       SSSSSSSSSS          TT
LLLLLLLLLLLL    EEEEEEEEEEEE    WW        WW       IIIIII        SSSSSSSS           TT

  SSSSSSSS      EEEEEEEEEEEE    VV        VV       IIIIII        GGGGGGGG      NN        NN
 SSSSSSSSSS     EEEEEEEEEEEE    VV        VV       IIIIII       GGGGGGGGGG     NNN       NN
SS        SS    EE               VV      VV          II        GG        GG    NNNN      NN
SSS       SS    EE               VV      VV          II        GG        GG    NNNNN     NN
 SSS            EE                VV    VV           II        GG              NN NNN    NN
   SSS          EEEEEEEE          VV    VV           II        GG              NN  NNN   NN
     SSS        EEEEEEEE           VV  VV            II        GG     GGGG     NN   NNN  NN
       SSS      EE                 VV  VV            II        GG     GGGG     NN    NNN NN
SS        SS    EE                  VVVV             II        GG        GG    NN     NNNNN
SS        SS    EE                  VVVV             II        GG        GG    NN      NNNN
 SSSSSSSSSS     EEEEEEEEEEEE         VV            IIIIII       GGGGGGGGGG     NN       NNN
  SSSSSSSS      EEEEEEEEEEEE         VV            IIIIII        GGGGGGGG      NN        NN

BBBBBBBBBB         IIIIII       NN        NN         222222         0000          888888
BBBBBBBBBBB        IIIIII       NNN       NN       2222222222     00000000       88888888
BB       BB          II         NNNN      NN      222      222   000    000     88      88
BB       BB          II         NNNNN     NN      22       222  000    00000    88      88
BB       BB          II         NN NNN    NN              222   00    00  00     88    88
BBBBBBBBBB           II         NN  NNN   NN             222    00   00   00      888888
BBBBBBBBBB           II         NN   NNN  NN           222      00  00    00    8888888888
BB       BB          II         NN    NNN NN         222        00 00     00   888      888
BB       BB          II         NN     NNNNN       222          0000     000   88        88
BB       BB          II         NN      NNNN       222           000    000    888      888
BBBBBBBBBBB        IIIIII       NN       NNN       222222222222   00000000      8888888888
BBBBBBBBBB         IIIIII       NN        NN       222222222222     0000         88888888

* * * * * * UNIVAC 1100 TIME/SHARING EXEC  ACCOUNT NUMBER * 1HPA01R50021 VER. EW 33R3HOST2 SITE *  HOST 2  * * * * * *

RUNID * LEWIST        USER ID *                 PART NUMBER * 00      INPUT DEVICE * CR1          OUTPUT DEVICE * PR2

  FILE NAME * PR@000LEWIST           CREATED AT:   12:51:12 OCT 15,1980           PRINTED AT:   13:27:53 OCT 15,1980

1234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890**SEQ NO. 07
```

```
@RUN LEWIST,1,F101R50021,SEVIGNBIN208,30,200

@MSG,N                    REMOVE AT CARD READER     10-15-80          CLOCK NO 2709

@ASG,T PUR,U9S,15753

@COPY,6 PUR.,TPF$.
FURPUR 28R1H1 E33 S74T11 10/15/80 13:04:46
SEVIGNBIN2CA*LEWIS(1) COPIED ON 09/18/80 AT 13:23:53
   105 BLOCKS COPIED.
EOF ENCOUNTERED ON INPUT TAPE

@XQT,A SYS$*MSFC$.LISTIT

@HDG,P      A

@PRT,S     A
FURPUR 28R1H1 E33 S74T11 10/15/80 13:05:53
```

```
A                                                                    DATE 101580        PAGE     1

SEVIGNBIN208*TPF$(0).A
            LIB LEWIS.,MIPS*ILIB.,SYS$*MSFC$.
            SEG DRIVER
            IN LEWIS.BLOCK1
            IN LEWIS.MAIN
            SEG 00*,(DRIVER)
            IN LEWIS.COALCV
            SEG 1*(DRIVER)
            IN LEWIS.SEARCH
            SEG 2*,(DRIVER)
            IN LEWIS.REACT
            SEG 3*(DRIVER)
            IN LEWIS.THERMP
            SEG 4*(DRIVER)
            IN LEWIS.DETON
            SEG 5*,(DRIVER)
            IN LEWIS.SHCK
            SEG 6*,(DRIVER)
            IN LEWIS.ROCKET

@HDG,P      BLOCK1
```

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OF POOR QUALITY

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BLOCK1                                                                                     DATE 101580          PAGE     1

@FOR,S    BLOCK1,BLOCK1
HSA  E3 -10/15/80-13:05:54 (11,)

    BLOCK DATA

    STORAGE USED: CODE(1) 000000; DATA(0) 000000; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003     CONSTS 000006
     0004     HOLCON 000010
     0005     MISC   001701
     0006     OUPT   000073

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0005    000640 AM         0005    000705 AM1        0005    001135 ANUM       0005 R 000004 ATAM       0005 R 000235 ATEM
     0003 R  000000 ATMN       0005    000004 AT04       0005    000514 BO         0005   000545 BOP        0005   000706 CPR1
     0005    000634 CPSUM      0005    000654 DATA       0005    001560 DENS       0004 R 000000 END        0005   001700 ENLSAV
     0005    000000 ENN        0005    001676 ENNL       0005    001677 ENSAVE     0005   001414 ENTH       0005   000636 EQRAT
     0006 R  000002 FA         0006 R  000003 FAP        0005    001445 FAZ        0006 R 000005 FB         0006 R 000006 FC
     0006 R  000007 FCP        0006 R  000012 FCST       0006 R  000014 FCV        0006 R 000015 FG         0006 R 000017 FGE
     0006 R  000020 FGV        0006 R  000021 FH         0006 R  000023 FI         0006 R 000025 FIV        0006 R 000027 FM
     0006 R  000031 FMT        0006 R  000050 FN         0006 R  000052 FOUR       0005   001527 FOX        0006 R 000053 FP
     0006 R  000054 FS         0006 R  000056 FSV        0006 R  000057 FT         0006 R 000061 FTK        0006 R 000063 FV
     0006 R  000065 FVEL       0006 R  000001 F13        0006 R  000000 F9X        0004 R 000001 GAS        0003 R 000001 GMET
     0005    000642 HPP        0005    000637 HSUBO      0004 I  000002 IE         0004 I 000003 IZERO      0004 I 000004 LANK
     0005    000463 LLMT       0004 I  000005 MOL        0005    000707 NAME       0005   000635 OF         0006 R 000067 ONE
     0004 R  000006 OX         0005    001644 OXF        0003 R  000002 PATM       0005   001363 PECWT      0005   000633 PP
     0003 R  000003 RBAR       0003 R  000004 RBR        0005    000644 RH         0005   001611 RHOP       0005   001612 RMW
     0005    001476 RTEMP      0003 R  000005 RVR        0005    000001 SUMN       0005   000003 SO         0005   000632 THIGH
     0006 R  000070 THREE      0005    001643 TLN        0005    000630 TLOW       0005   000627 TM         0005   000631 TMID
     0005    000002 TT         0006 R  000071 TWO        0005    000646 VMIN       0005   000650 VPLS       0005   000652 WP
     0004 R  000007 ZERO       0006 R  000072 ZEROF


 00101        1*            BLOCK DATA                                                                  ATM00001      000000
 00101        2*      C                                                                                               000000
 00102        3*            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                                  /CONSTS/      000000
 00103        4*            COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                            /HOLCON/      000000
 00104        5*            COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                                000000
 00104        6*          1               BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                              000000
 00104        7*          2               HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),                /MISC/        000000
 00104        8*          3               DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),                           000000
 00104        9*          4               ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,                            000000
 00104       10*          5               RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                                       000000
 00105       11*            COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),              /OUPT/        000000
 00105       12*          1               FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR,           /OUPT/        000000
 00105       13*          2               FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,             /OUPT/        000000
 00105       14*          3               TWO,ZEROF                                                      /OUPT/        000000
 00105       15*      C                                                                                               000000
 00106       16*            DIMENSION ATAM(3,51),ATEM(3,50)                                                           000000
 00107       17*            EQUIVALENCE (ATOM(1,1),ATAM),(ATOM(1,52),ATEM)                                            000000
```

```
00107    18*    C                                                                           000000
00107    19*    C  ATOMIC SYMBOLS, WEIGHTS, AND VALENCES                                    000000
00110    20*          DATA ATAM/2HH ,1.00797,1.0,2HHE,4.0026,0.0,2HLI,6.939,1.0,2HBE,       000000
00110    21*        1 9.0122,2.0,2HB ,10.811,3.0,2HC ,12.01115,4.0,2HN ,14.0067,0.0,        000000
00110    22*        2 2HO ,15.9994,-2.0,2HF ,18.9984,-1.0,2HNE,20.183,0.0,2HNA,22.9898      000000
00110    23*        3 1.0,2HMG,24.312,2.0,2HAL,26.9815,3.0,2HSI,28.086,4.0,2HP ,30.9738     000000
00110    24*        4,5.0,2HS ,32.064,4.0,2HCL,35.453,-1.0,2HAR,39.948,0.0,2HK ,39.102,     000000
00110    25*        5 1.0,2HCA,40.080,2.0,2HSC,44.956,3.0,2HTI,47.90,4.0,2HV ,50.942,       000000
00110    26*        6 5.0,2HCR,51.996,3.0,2HMN,54.9380,2.0,2HFE,55.847,3.0,2HCO,58.9332     000000
00110    27*        7,2.0,2HNI,58.710,2.0,2HCU,63.540,2.0,2HZN,65.370,2.0,2HGA,69.720,      000000
00110    28*        8 3.0,2HGE,72.590,4.0,2HAS,74.9216,3.0,2HSE,78.960,4.0,2HBR,79.909,     000000
00110    29*        9 -1.0,2HKR,83.80,0.0,2HRB,85.47,1.0,2HSR,87.620,2.0,2HY ,88.905,       000000
00110    30*        A 3.0,2HZR,91.220,4.0,2HNB,92.906,5.0,2HMO,95.94,6.0,2HTC,99.0,7.0,     000000
00110    31*        B 2HRU,101.070,3.0,2HRH,102.905,3.0,2HPD,106.40,2.0,2HAG,107.870,       000000
00110    32*        C 1.0,2HCD,112.40,2.0,2HIN,114.820,3.0,2HSN,118.690,4.0,2HSB,           000000
00110    33*        D 121.750,3.0/                                                          000000
00112    34*          DATA ATEM/2HTE,127.60,4.0,2HI ,126.9044,-1.0,2HXE,131.30,0.0,2HCS,    000000
00112    35*        1 132.905,1.0,2HBA,137.340,2.0,2HLA,138.910,3.0,2HCE,140.120,3.0,       000000
00112    36*        2 2HPR,140.907,3.0,2HND,144.240,3.0,2HPM,145.0,3.0,2HSM,150.350,3.0     000000
00112    37*        3,2HEU,151.960,3.0,2HGD,157.250,3.0,2HTB,158.924,3.0,2HDY,162.50,       000000
00112    38*        4 3.0,2HHO,164.930,3.0,2HER,167.260,3.0,2HTM,168.934,3.0,2HYB,          000000
00112    39*        5 173.040,3.0,2HLU,174.997,3.0,2HHF,178.490,4.0,2HTA,180.948,5.0,       000000
00112    40*        6 2HW ,183.850,6.0,2HRE,186.20,7.0,2HOS,190.20,4.0,2HIR,192.20,4.0,     000000
00112    41*        7 2HPT,195.090,4.0,2HAU,196.967,3.0,2HHG,200.590,2.0,2HTL,204.370,      000000
00112    42*        8 1.0,2HPB,207.190,2.0,2HBI,208.980,3.0,2HPO,210.0,2.0,2HAT,210.0,      000000
00112    43*        9 0.0,2HRN,222.0,0.0,2HFR,223.0,1.0,2HRA,226.0,2.0,2HAC,227.0,3.0,      000000
00112    44*        A 2HTH,232.038,4.0,2HPA,231.0,5.0,2HU ,238.030,6.0,2HNP,237.0,5.0,      000000
00112    45*        B 2HPU,242.0,4.0,2HAM,243.0,3.0,2HCM,247.0,3.0,2HBK,249.0,3.0,2HCF,     000000
00112    46*        C 251.0,3.0,2HES,254.0,0.0,2HFM,253.0,0.0,2HIC,12.01115,4.0/            000000
00112    47*    C     INFORMATION USED IN VARIABLE OUTPUT FORMAT                            000000
00114    48*          DATA F9X/3H9X,/,F13/2H13/,FA/6HAE/AT /,FB/6H      /,FC/6HCF    /, /OUPT/  000000
00114    49*        1     FCV/6HCF VAC/,FG/12HGAMMA (S)   /,FI/12HISP SECONDS /,       /OUPT/  000000
00114    50*        2     FIV/12HIVAC SECONDS/,FM/12HM MOL WEIGHT/,FMT/6H(1H ,2,       /OUPT/  000000
00114    51*        3     6HA6,A2,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,    /OUPT/  000000
00114    52*        4     5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1)/,    /OUPT/  000000
00114    53*        5     FN/12HMACH NUMBER /,FOUR/5HF9.4,/,FP/6HPC/P  /,              /OUPT/  000000
00114    54*        6     FT/12H(DLV/DLP) T /,FV/12H(DLV/DLT) P /,ONE/5HF9.1,/,        /OUPT/  000000
00114    55*        7     THREE/5HF9.3,/,TWO/5HF9.2,/,ZEROF/5HF9.0,/,FAP/12HPRESS N/M**         000000
00114    56*        82/,FCP/12HCP CAL/(G)(K,2H) /,FCST/12HCSTAR M/SEC /,FGE/6H(EFF) /,          000000
00114    57*        9 FGV/6HGAS VE/,FH/12HENTH CAL/G  /,FS/12HS CAL/(G)(K)/,FSV/6HSON V         000000
00114    58*        AE/,FTK/12HTEMP DEG. K /,FVEL/6HL M/SE,2HC /                                000000
00153    59*          DATA END/3HEND/,GAS/1HG/,IE/1HE/,IZERO/2H00/,LANK/2H  /,MOL/1HM/          000000
00153    60*        1 ,OX/1HO/,ZERO/1H0/,ATMN/101325.0/,RVR/82.0554497/                         000000
00153    61*        3 ,GMET/9.806650/,PATM/14.6960060/,RBAR/1.9871650/,RBR/8314.298360/         000000
00172    62*          END                                                          ATM00060     000000

      END OF COMPILATION:        NO  DIAGNOSTICS,


@HDG,P      BOOT


@PRT,S     BOOT
FURPUR 28R1H1 E33 S74T11 10/15/80 13:05:56
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```
SEVIGNBIN208*TPF$(0).BOOT
        @CAT,P LEWIS,F/64/TRK/128
        @CAT,P 4,F/64/TRK/1.
        @CAT,P 8,F/10/TRK/32
        @CAT,P 10,F/10/TRK/32
        @CAT,P 12,F/10/TRK/64
        @ASG,A LEWIS.
        @ASG,A 4.
        @ASG,A 8.
        @ASG,A 10.
        @ASG,A 12.
        @COPY TPF$.,LEWIS.
        @COPY,G PUR.,4.
        @COPY,G PUR.,8.
        @COPY,G PUR.,10.
        @COPY,G PUR.,12.
        @FREE PUR.

@HDG,P        CHECK
```

```
   CHECK                                                                                      DATE 101580        PAGE      1

aFOR,S     CHECK,CHECK
HSA  E3 -10,15/80-13:05:57 (2,)

   SUBROUTINE CHECK       ENTRY POINT 000056

   STORAGE USED: CODE(1) 000065; DATA(0) 000013; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003   NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000 I 000000 IBLNK2    0000 I 000005 ICHAR1    0000 I 000006 ICHAR2    0000 I 000001 IHIGH    0000 I 000002 ILOW
    0000   000007 INJP$     0000 I 000003 JHIGH     0000 I 000004 JLOW


00101       1*              SUBROUTINE CHECK(NAME)                                                         000000
00101       2*      C                                                                                      000000
00101       3*      C       BLANK FILL SPECIES SYMBOLS                                                     000000
00103       4*              DATA IBLNK2/2H  /,IHIGH/1HZ/,ILOW/1HA/                                         000000
00107       5*              DATA JHIGH/0/,JLOW/0/ ,ICHAR1/0/,ICHAR2/0/                                     000000
00114       6*              FLD(30,6,ICHAR1)=FLD(0,6,NAME)                                                 000000
00115       7*              FLD(30,6,ICHAR2)=FLD(6,6,NAME)                                                 000001
00116       8*              FLD(30,6,JHIGH)=FLD(0,6,IHIGH)                                                 000003
00117       9*              FLD(30,6,JLOW)=FLD(0,6,ILOW)                                                   000005
00120      10*              IF(ICHAR1.LT.JLOW .OR. ICHAR1.GT.JHIGH) NAME=IBLNK2                            000007
00122      11*              IF(ICHAR2.LT.JLOW .OR. ICHAR1.GT.JHIGH) FLD(6,6,NAME)=                         000027
00122      12*          *   FLD(6,6,IBLNK2)                                                                000027
00124      13*              RETURN                                                                         000047
00125      14*              END                                                                            000064

      END OF COMPILATION:          NO  DIAGNOSTICS.

aHDG,P       COALCV
```

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OF POOR QUALITY

```
@FOR,S    COALCV,COALCV
HSA  E3 -10/15/80-13:05:59 (24,)

   SUBROUTINE COALCV     ENTRY POINT 003674

   STORA   USED: CODE(1) 003713; DATA(0) 003744; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CFUEL   000004
    0004    SPECES  017106
    0005    INDX    000021
    0006    CCC     000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0007    RDYES
    0010    PAGIT
    0011    CHRSIZ
    0012    GOUT
    0013    NNCOD$
    0014    RDATAI
    0015    RDATAF
    0016    NREW$
    0017    NRBU$
    0020    NIO2$
    0021    NIO3$
    0022    NIO1$
    0023    NERR2$
    0024    NWBU$
    0025    NWEF$
    0026    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    000030 10L        0000    002175 100F       0001    001444 1011G      0001    001477 1025G      0001    000460 104L
    0001    001535 1040G      0000    002205 106F       0001    001743 1073G      0000    002233 108F       0001    001764 1107G
    0001    000537 112L       0001    002063 1137G      0001    000554 114L       0001    002075 1147G      0001    000607 120L
    0001    002213 1204G      0001    002213 1207G      0001    002246 1225G      0001    002316 1245G      0001    000617 126L
    0001    002360 1270G      0001    002370 1273G      0001    000635 130L       0001    002454 1322G      0001    002531 1347G
    0001    002541 1354G      0001    002553 1362G      0001    002565 1370G      0001    002576 1375G      0001    002607 1405G
    0001    002653 1426G      0001    002733 1452G      0001    002734 1455G      0001    003021 1504G      0001    003034 1511G
    0001    003035 1514G      0001    003213 1550G      0001    003214 1553G      0001    003253 1574G      0001    003263 1577G
    0001    003322 1615G      0001    003407 1642G      0001    003422 1647G      0001    003423 1652G      0001    003564 1727G
    0001    003564 1731G      0001    003571 1736G      0001    003571 1740G      0001    003576 1745G      0001    003576 1747G
    0001    003603 1754G      0001    003603 1756G      0001    003620 1770G      0001    003624 1774G      0001    000011 205G
    0001    000016 212G       0000    002404 2350F      0001    001102 2352L      0000    002410 2354F      0001    001137 2357L
    0001    001143 2358L      0001    001177 2360L      0001    001250 2364L      0001    001254 2366L      0001    001257 2370L
    0001    001263 2372L      0001    001315 2380L      0001    001352 2386L      0001    002053 2420L      0001    002116 2422L
    0000    002547 2424F      0001    002112 2427L      0001    002152 2428L      0001    002216 2431L      0001    002222 2432L
    0001    002225 2434L      0001    002231 2436L      0001    000126 256G       0001    000126 260G       0001    000133 265G
    0001    000133 267G       0001    000140 274G       0001    000140 276G       0001    000637 300L       0001    000145 303G
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0001     000145 305G     0001     000643 310L     0001     000660 312L     0001     000675 314L     0001     000677 316L
0001     000710 320L     0001     000716 322L     0001     000727 324L     0001     000740 326L     0001     000751 328L
0001     000762 330L     0001     000773 340L     0001     001013 342L     0001     000240 343G     0001     001017 343L
0001     001060 348L     0001     001063 350L     0001     001356 351L     0001     001366 352L     0001     001377 354L
0001     001410 356L     0001     001421 358L     0001     000273 362G     0001     001502 364L     0001     001520 366L
0001     001524 367L     0001     000302 370G     0001     001562 372L     0001     001565 380L     0001     001567 382L
0001     001600 390L     0000     002533 394F     0001     001773 400L     0001     002020 402L     0001     000335 406G
0001     000343 413G     0001     002031 420L     0001     002267 421L     0001     002301 422L     0001     002305 423L
0001     002347 428L     0001     002352 430L     0001     002405 434L     0001     002410 440L     0001     002412 442L
0001     000434 445G     0001     002423 450L     0001     002437 452L     0001     002443 453L     0001     000444 454G
0001     002501 460L     0001     002504 470L     0001     000160 50L      0001     000515 500G     0001     002706 504L
0001     000523 505G     0001     002767 520L     0001     000611 533G     0001     003070 540L     0001     000626 543G
0001     003276 552L     0001     003301 554L     0000     002020 56F      0001     003361 560L     0000     002024 58F
0001     003455 590L     0000     002032 60F      0000     002055 62F      0001     001030 620G     0001     001112 654G
0001     001122 662G     0001     003652 680L     0000     002100 70F      0001     001245 717G     0001     001245 722G
0001     001300 740G     0001     001323 751G     0001     001334 754G     0001     000316 80L      0000     002122 84F
0001     000357 90L      0000     002131 92F      0000     002143 96F      0004     011052 A        0000 R 003331 ACOMP
0000 R 000576 ANUM       0000 R 003461 ASH        0000 R 001776 ASHF       0000 R 001640 CC         0000 R 002744 CCOMP
0003 R 000000 CF         0000 R 002732 COAL       0004     000000 COEF     0005     000001 CONVG    0000 R 001774 CSUM
0000 R 001760 CTEMP      0004     010624 DELN     0006     000002 DEMAND   0000 R 001562 DENS       0004     004312 EN
0004     010150 ENLN     0000 R 001447 ENTH       0000 R 002676 FAZ        0000 R 001766 FES2       0000 R 002000 FES2C
0000 R 001531 FOX        0006     000000 GRAPH    0000 R 002001 HF1        0000 R 002003 HF2        0000 R 001734 HH
0000 R 001664 HHT        0000 R 001777 HHV        0003 R 000001 HHVV       0005     000003 HP       0004     010376 HO
0000 R 001657 H2O        0000 I 001637 I          0000 I 003331 IACOMP     0000 I 003461 IASH       0000 I 001744 IC
0000 I 001645 ICC        0000 I 002744 ICCOMP     0000 I 002732 ICOAL      0000 I 001625 ID         0005     000000 IDEBUG
0000 I 001752 IE         0000 I 002676 IFAZ       0000 I 001652 IH2O       0005     000015 IMAT     0000     003713 INJPS
0000 I 003040 IOFUEL     0000 I 001746 IOPT       0000 I 001760 IOUT       0000 I 003242 IOXID      0000 I 002727 IPROX
0005     000016 IQ1      0005     000005 ISV      0004     016266 IUSE     0000 I 001757 J          0000 I 001761 JJ
0000 I 001613 JOPT       0006     000001 JOUT     0005     000014 KMAT     0000 I 001763 KOUT       0005     000012 L
0000 I 000000 LINE1      0000 I 001767 LL         0000 I 001764 LN         0000 I 001765 L1         0000 I 001416 MOLE
0005     000006 MOLES    0000 I 001772 N          0000 I 000007 NAME       0000 I 001754 NASH       0000 I 001753 NCOAL
0000 I 001747 NDUMMY     0000 I 001755 NFUEL      0000 I 001762 NI         0005     000017 NOF      0005     000020 NOMIT
0000 I 001756 NOXID      0005     000007 NP       0005     000011 NPT      0000 I 001745 NREAC      0005 I 000013 NS
0005     000010 NT       0000 R 003040 OFUEL      0004 I 010150 OMIT       0000 R 001751 OTEMP      0000 R 003242 OXID
0000 R 001365 PECWT      0003 R 000003 PER        0000 R 002727 PROX       0000 R 002002 PX         0007 L 000000 RDYES
0000 R 001632 RMOL       0000 R 001500 RTEMP      0004     004064 S        0000 R 001770 SINRT      0004     016660 SLN
0005     000004 SP       0004     015364 SUB      0000 R 001771 SUM        0000 R 001773 SUM1       0000 R 001775 SUM2
0000 R 002004 SUM3       0004     016514 TEMP     0005     000002 TP       0003 R 000002 WCR


00101      1*              SUBROUTINE COALCV(FIRST)                                                000000
00101      2*        C        USE MIPS INPUT ROUTINES TO READ COAL CONVERSION                      000000
00101      3*        C              AND CREATE SIMULATED REACTANT CARDS                            000000
00103      4*              COMMON /CFUEL/CF,HHVV,WCR,PER                                           000000
00104      5*              COMMON /SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)        000000
00104      6*             X   ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)        000000
00105      7*              COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,            000000
00105      8*             X   KMAT,IMAT,IQ1,NOF,NOMIT                                              000000
00106      9*              COMMON /CCC/GRAPH,JOUT,DEMAND                                           000000
00107     10*              INTEGER OMIT                                                            000000
00110     11*              DIMENSION OMIT(3,50)                                                    000000
00111     12*              EQUIVALENCE (OMIT(1,1),ENLN(1))                                         000000
00112     13*              LOGICAL FIRST,RDYES                                                     000000
00113     14*              DIMENSION LINE1(7)                                                      000000
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00114     15*        DATA LINE1/42H TYPE YES TO READ IN PREVIOUS COMPOSITION /                    000000
00114     16*   C    DATA ARRAYS FOR REACTANT CARDS                                                000000
00116     17*        DIMENSION NAM (15,25),ANUM(15,25),PECWT(25),MOLE(25),ENTH(25),                000000
00116     18*      X    FAZ(25),PTEMP(25),FOX(25),DENS(25)                                         000000
00117     19*        DIMENSION IFAZ(15)                                                            000000
00120     20*        EQUIVALENCE (FAZ(1),IFAZ(1))                                                  000000
00120     21*   C    ARRAYS FOR COAL DATA                                                          000000
00121     22*        DIMENSION IPROX(3)                                                            000000
00122     23*        DIMENSION PROX(3),COAL(5,2),ICOAL(5,2),CCOMP(12,5),ICCOMP(12,5),              000000
00122     24*      X    OFUEL(13,10),IOFUEL(13,10),OXID(11,5),IOXID(11,5),                         000000
00122     25*      X    ACOMP(11,8),IACOMP(11,8)                                                   000000
00123     26*        EQUIVALENCE (PROX(1),IPROX(1))                                                000000
00124     27*        EQUIVALENCE (COAL(1,1),ICOAL(1,1))                                            000000
00125     28*        EQUIVALENCE (CCOMP(1,1),ICCOMP(1,1))                                          000000
00126     29*        EQUIVALENCE (OFUEL(1,1),IOFUEL(1,1))                                          000000
00127     30*        EQUIVALENCE (OXID(1,1),IOXID(1,1))                                            000000
00130     31*        EQUIVALENCE (ACOMP(1,1),IACOMP(1,1))                                          000000
00131     32*        DIMENSION JOPT(10)                                                            000000
00132     33*        DIMENSION ID(5),RMOL(5)                                                       000000
00133     34*        DATA (ID(I),I=1,5)/'C','H','N','O','S'/                                       000000
00135     35*        DATA (RMOL(I),I=1,5)/12.01115,1.00797,14.0067,15.994,32.064/                  000000
00137     36*        DIMENSION ASH(10,5),IASH(10,5)                                                000000
00140     37*        EQUIVALENCE (ASH(1,1),IASH(1,1))                                              000000
00141     38*        DATA (IASH(I,1),I=1,10,2)/'SI','O',3*' '/                                     000000
00143     39*        DATA (IASH(I,2),I=1,10,2)/'FE','O',3*' '/                                     000000
00145     40*        DATA (IASH(I,3),I=1,10,2)/'AL','O',3*' '/                                     000000
00147     41*        DATA (IASH(I,4),I=1,10,2)/'FE','S',3*' '/                                     000000
00151     42*        DATA (ASH(I,1),I=2,10,2)/1.,2.,3*0./                                          000000
00153     43*        DATA (ASH(I,2),I=2,10,2)/2.,3.,3*0./                                          000000
00155     44*        DATA (ASH(I,3),I=2,10,2)/2.,3.,3*0./                                          000000
00157     45*        DATA (ASH(I,4),I=2,10,2)/1.,2.,3*0./                                          000000
00161     46*        DIMENSION CC(5),ICC(5)                                                        000000
00162     47*        DATA (ICC(I),I=1,5)/'C   ',4*' '/                                             000000
00164     48*        DATA (CC(I),I=1,5)/1.,4*0./                                                   000000
00166     49*        DIMENSION IH2O(5),H2O(5)                                                      000000
00167     50*        DATA (IH2O(I),I=1,5)/'H','O',3*' '/                                           000000
00171     51*        DATA (H2O(I),I=1,5)/2.,1.,3*0./                                               000000
00173     52*        DIMENSION HHT(40),HH(8)                                                       000000
00174     53*        DATA (HHT(I),I=1,40)/                                                         000000
00174     54*      X' 0 - E','NTER D','ATA   ',2*'      ',                                        000000
00174     55*      X' 1 - D','ULONG ','1     ',2*'      ',                                        000000
00174     56*      X' 2 - D','ULONG ','2     ',2*'      ',                                        000000
00174     57*      X' 3 - C','PP2   ',3*'      ',                                                  000000
00174     58*      X' 4 - G','RUMMEL','-DAVIS',2*'      ',                                        000000
00174     59*      X' 5 - C','CSTOB ',3*'      ',                                                 000000
00174     60*      X' 6 - M','AX OF ','ABOVE ',2*'      ',                                        000000
00174     61*      X' 7 - M','IN OF ','ABOVE ',2*'      '                                         000000
00174     62*      X    /                                                                          000000
00176     63*        DATA IC/12/                                                                   000000
00200     64*        CALL PAGIT                                                                    000000
00201     65*        CALL CHRSIZ(4)                                                                000001
00202     66*        NREAC=0                                                                       000004
00203     67*        IOPT=0                                                                        000005
00204     68*        DO 2 I=1,10                                                                   000011
00207     69*      2 JOPT(I)=1                                                                     000011
00211     70*        DO 12 I=1,5                                                                   000016
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      COALCV                                                                                DATE 101580        PAGE    4

00214     71*         12 ICOAL(I,1)=ID(I)                                                  000016
00214     72*     C      FOR FIRST PASS DO NOT CHECK SAVED DATA                            000016
00216     73*            IF (.NOT.FIRST) GO TO 10                                          000020
00220     74*            IF (.NOT.RDYES(LINE1,42)) GO TO 300                               000022
00222     75*         10 CONTINUE                                                          000030
00222     76*     C      READ IN PREVIOUS COAL DATA                                        000030
00223     77*            REWIND IC                                                         000030
00224     78*            READ (IC) NDUMMY,CF,HHVV,WCR,PER                                  000032
00233     79*            READ (IC) CTEMP,OTEMP                                             000043
00237     80*            READ (IC) PROX,COAL,PER,IE,HH                                     000051
00246     81*            READ (IC) NCOAL,NASH,NFUEL,NOXID                                  000071
00254     82*            READ (IC) ((CCOMP(I,J),I=1,12),J=1,NCOAL),                        000112
00254     83*           X    ((ACOMP(I,J),I=1,11),J=1,NASH),                                000112
00254     84*           X    ((OFUEL(I,J),I=1,13),J=1,NFUEL),                               000112
00254     85*           X    ((OXID(I,J),I=1,11),J=1,NOXID)                                 000112
00254     86*     C      DISPLAY PRESENT COAL DATA                                         000112
00312     87*            IF (FIRST) GO TO 50                                               000150
00314     88*            IF (.NOT.RDYES(LINE1,42)) GO TO 300                               000152
00316     89*         50 CONTINUE                                                          000160
00317     90*            CALL GOUT(' 1 - VOLATILE (OPTIONAL) AND ASH AS LBS/100 LBS DRY COA  000160
00317     91*           XL',56)                                                             000160
00320     92*            ENCODE (56,IOUT) PROX(1)                                          000163
00323     93*         56 FORMAT (6X,'VOLATILE',F10.4)                                      000171
00324     94*            CALL GOUT(IOUT,24)                                                000171
00325     95*            ENCODE (58,IOUT) PROX(3)                                          000175
00330     96*         58 FORMAT (6X,'ASH',5X,F10.4)                                        000203
00331     97*            CALL GOUT(IOUT,24)                                                000203
00332     98*            CALL GOUT(' ',1)                                                  000207
00333     99*            ENCODE (60,IOUT) CTEMP                                            000213
00336    100*         60 FORMAT (' 2 - COAL TEMPERATURE IN DEG F',F10.2)                   000221
00337    101*            CALL GOUT(IOUT,40)                                                000221
00340    102*            CALL GOUT(' ',1)                                                  000225
00341    103*            CALL GOUT(' 3 - DRY COAL COMPOSITION AS LBS/100 LBS DRY COAL',49)  000231
00342    104*            DO 66 I=1,5                                                       000240
00345    105*            ENCODE (62,IOUT) ICOAL(I,1),COAL(I,2)                             000240
00351    106*         62 FORMAT (5X,A4,5X,F10.4)                                           000246
00352    107*            CALL GOUT(IOUT,24)                                                000246
00353    108*         66 CONTINUE                                                          000253
00355    109*            CALL GOUT(' ',1)                                                  000253
00356    110*            CALL GOUT(' 4 - OTHER COAL COMPONENTS AS LBS/100 LBS DRY COAL, STA  000257
00356    111*           XTE AND COMPOSITION',73)                                            000257
00357    112*            IF (NCOAL.EQ.0) GO TO 80                                          000263
00361    113*            DO 72 I=1,NCOAL                                                   000265
00364    114*            ENCODE (70,IOUT) CCOMP(1,I),ICCOMP(2,I),                          000273
00364    115*           X    (ICCOMP(J*2+1,I),CCOMP(J*2+2,I),J=1,5)                         000273
00375    116*         70 FORMAT (F10.4,10X,A4,5(2X,A2,2X,F8.4))                            000306
00376    117*            CALL GOUT(IOUT,94)                                                000306
00377    118*         72 CONTINUE                                                          000316
00401    119*         80 CALL GOUT(' ',1)                                                  000316
00402    120*            CALL GOUT(' 5 - ASH COMPOSITION AS LBS/100 LBS ASH AND COMPONENT',  000321
00402    121*           X    53)                                                            000321
00403    122*            IF (NASH.EQ.0) GO TO 90                                           000325
00405    123*            DO 88 I=1,NASH                                                    000327
00410    124*            ENCODE (84,IOUT) ACOMP(1,I),(IACOMP(J*2,I),ACOMP(J*2+1,I),J=1,5)  000335
00420    125*         84 FORMAT (F10.4,14X,5(2X,A2,2X,F8.4))                               000347
00421    126*            CALL GOUT(IOUT,94)                                                000347
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00422            88 CONTINUE                                                    000357
00424            90 CALL GOUT(' ',1)                                            000357
00425               ENCODE (92,IOUT) PER                                        000362
00430            92 FORMAT (' 6 - FRACTION CARBON CONVERSION',F10.4)            000370
00431               CALL GOUT(IOUT,41)                                          000370
00432               CALL GOUT(' ',1)                                            000374
00433               ENCODE (96,IOUT) HH(IE+1)                                   000400
00436            96 FORMAT (' 7 - HEATING VALUE OF COAL BTU/LB',F13.3)          000410
00437               CALL GOUT(IOUT,46)                                          000410
00440               CALL GOUT(' ',1)                                            000414
00441               CALL GOUT(' 8 - OTHER FUEL COMPONENTS AS LBS/LB COAL, TEMPERATURE 000420
00441              XIN DEG F, STATE AND COMPOSITION',86)                        000420
00442               IF (NFUEL.EQ.0) GO TO 104                                   000424
00444               DO 102 I=1,NFUEL                                            000426
00447               ENCODE (100,IOUT) OFUEL(1,I),OFUEL(2,I),IOFUEL(3,I),        000434
00447              X    (IOFUEL(J*2+2,I),OFUEL(J*2+3,I),J=1,5)                  000434
00461           100 FORMAT (F10.4,F10.3,1X,A3,5(2X,A2,2X,F8.4))                 000450
00462               CALL GOUT(IOUT,94)                                          000450
00463           102 CONTINUE                                                    000460
00465           104 CALL GOUT(' ',1)                                            000460
00466               ENCODE (106,IOUT) OTEMP                                     000463
00471           106 FORMAT (' 9 - OXIDIZER TEMPERATURE IN DEG F',F10.2)         000471
00472               CALL GOUT(IOUT,44)                                          000471
00473               CALL GOUT(' ',1)                                            000475
00474               CALL GOUT(' 10 - OXIDIZER COMPONENTS AS LBS/100 LBS OXIDIZER AND C 000501
00474              XOMPONENT',63)                                               000501
00475               IF (NOXID.EQ.0) GO TO 112                                   000505
00477               DO 110 I=1,NOXID                                            000507
00502               ENCODE (108,IOUT) OXID(1,I),(IOXID(J*2,I),OXID(J*2+1,I),J=1,5) 000515
00512           108 FORMAT (F10.4,14X,5(2X,A2,2X,F8.4))                         000527
00513               CALL GOUT(IOUT,94)                                          000527
00514           110 CONTINUE                                                    000537
00516           112 CALL GOUT(' ',1)                                            000537
00517               CALL GOUT(' TYPE 1 OR 2 TO MODIFY OR REPLACE',33)           000542
00520               CALL GOUT('     RETURN TO CONTINUE',23)                     000546
00521               IOPT=0                                                      000552
00522           114 CONTINUE                                                    000554
00523               CALL RDATAI(1,IOPT,$114)                                    000554
00524               IF (IOPT.LT.0.OR.IOPT.GT.2) GO TO 114                       000560
00526               IF (IOPT.EQ.0) GO TO 680                                    000575
00530               GO TO (120,300),IOPT                                        000577
00530         C     SELECT GROUPS TO BE CHANGED                                 000577
00531           120 CONTINUE                                                    000611
00532               DO 124 I=1,10                                               000611
00535           124 JOPT(I)=0                                                   000611
00537               CALL GOUT (' TYPE GROUP NUMBERS OF DATA TO BE CHANGED IN ASCENDING 000612
00537              X ORDER.   FOR EXAMPLE 1 3 7 9',83)                          000612
00540           126 CONTINUE                                                    000617
00541               CALL RDATAI(10,JOPT,$126)                                   000617
00542               DO 130 I=10,1,-1                                            000626
00545               JJ=JOPT(I)                                                  000626
00546               IF (JJ.EQ.0) GO TO 130                                      000627
00550               JOPT(I)=0                                                   000631
00551               JOPT(JJ)=JJ                                                 000633
00552           130 CONTINUE                                                    000637
00552         C     ADD OR UPDATE COAL DATA                                     000637
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00554     183*      300 CONTINUE                                                               000637
00555     184*          CALL PAGIT                                                             000637
00556     185*          IF (JOPT(1).EQ.0) GO TO 314                                            000640
00556     186*      C   READ IN PROXIMATE ANALYSIS DATA                                        000640
00560     187*      310 CALL GOUT(' TYPE (OPTIONAL) LBS VOLATILES/100 LBS DRY COAL',47)        000643
00561     188*          CALL RDATAF(1,PROX(1),$310)                                            000646
00562     189*          IF (IPROX(1).EQ.'        ') PROX(1)=0.                                 000653
00564     190*      312 CALL GOUT(' TYPE LBS ASH/100 LBS DRY COAL',30)                         000660
00565     191*          CALL RDATAF(1,PROX(3),$312)                                            000663
00566     192*          PROX(2)=100.-PROX(1)-PROX(3)                                           000670
00567     193*      314 IF (JOPT(2).EQ.0) GO TO 320                                            000675
00567     194*      C   READ IN COAL TEMPERATURE                                               000675
00571     195*      316 CALL GOUT(' TYPE COAL TEMPERATURE IN DEG F',31)                        000677
00572     196*          CALL RDATAF(1,CTEMP,$316)                                              000702
00573     197*      320 IF (JOPT(3).EQ.0) GO TO 340                                            000710
00573     198*      C   READ IN REACTING COAL COMPOSITION                                      000710
00575     199*          CALL GOUT(' TYPE LBS/100 LBS DRY COAL FOR ELEMENTS',39)                000711
00576     200*      322 CALL GOUT(' C',2)                                                      000716
00577     201*          CALL RDATAF(1,COAL(1,2),$322)                                          000721
00600     202*      324 CALL GOUT(' H',2)                                                      000727
00601     203*          CALL RDATAF(1,COAL(2,2),$324)                                          000732
00602     204*      326 CALL GOUT(' N',2)                                                      000740
00603     205*          CALL RDATAF(1,COAL(3,2),$326)                                          000743
00604     206*      328 CALL GOUT(' O',2)                                                      000751
00605     207*          CALL RDATAF(1,COAL(4,2),$328)                                          000754
00606     208*      330 CALL GOUT(' S',2)                                                      000762
00607     209*          CALL RDATAF(1,COAL(5,2),$330)                                          000765
00610     210*      340 IF (JOPT(4).EQ.0) GO TO 350                                            000773
00610     211*      C   READ IN OTHER COAL COMPONENTS                                          000773
00612     212*          CALL GOUT(' TYPE (OPTIONAL) OTHER COAL COMPONENTS',38)                 000774
00613     213*          CALL GOUT(' TYPE LBS/100 LBS DRY COAL,STATE AND AND COMPONENT',50)     001000
00614     214*          CALL GOUT(' COAL TEMPERATURE IS ASSUMED',28)                           001004
00615     215*          NI=1                                                                   001010
00616     216*      342 CALL GOUT('     EXAMPLE 0.13  1HG  2HCL  2.',32)                       001013
00617     217*      343 DO 344 J=1,5                                                           001017
00622     218*          ICCOMP(J*2+1,NI)=2H                                                    001030
00623     219*      344 CCOMP(J*2+2,NI)=0.                                                     001031
00625     220*          CCOMP(1,NI)=0.                                                         001033
00626     221*          ICCOMP(2,NI)='        '                                                001035
00627     222*      346 CALL RDATAF(12,CCOMP(1,NI),$342)                                       001037
00630     223*          IF (CCOMP(1,NI)) ,348,                                                 001046
00633     224*          IF (ICCOMP(1,NI).EQ.'        ') GO TO 348                              001050
00635     225*          NI=NI+1                                                                001053
00636     226*          GO TO 343                                                              001056
00637     227*      348 NCOAL=NI-1                                                             001060
00640     228*      350 IF (JOPT(5).EQ.0) GO TO 380                                            001063
00642     229*          IF (IOPT.NE.1) GO TO 351                                               001064
00644     230*          ENCODE (2350,IOUT) JOPT(5)                                             001067
00647     231*     2350 FORMAT (' GROUP NUMBER',I5)                                            001075
00650     232*          CALL GOUT(IOUT,18)                                                     001075
00651     233*     2352 IF (NASH.EQ.0) GO TO 2357                                              001102
00653     234*          DO 2356 I=1,NASH                                                       001103
00656     235*          ENCODE (2354,IOUT) I,ACOMP(1,I),                                       001112
00656     236*         X   (IACOMP(J*2,I),IACOMP(J*2+1,I),J=1,5)                               001112
00667     237*     2354 FORMAT (I4,F10.4,14X,5(2X,A2,2X,F8.4))                                 001126
00670     238*          CALL GOUT(IOUT,98)                                                     001126
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00671    239*      2356 CONTINUE                                                                          001137
00673    240*      2357 CALL GOUT(' TYPE 1-ALTER, 2-DELETE, 3-ADD, RETURN TO CONTINUE',50)               001137
00674    241*      2358 KOUT=0                                                                            001143
00675    242*           CALL RDATAI(1,KOUT,$2358)                                                         001143
00676    243*           IF (KOUT.LT.0.OR.KOUT.GT.3) GO TO 2358                                            001150
00700    244*           IF (KOUT.EQ.0) GO TO 2380                                                         001165
00702    245*           IF (KOUT.EQ.3) GO TO 2370                                                         001167
00704    246*           CALL GOUT(' TYPE LINE NUMBER.',17)                                                001172
00705    247*      2360 LN=0                                                                              001177
00706    248*           CALL RDATAI(1,LN,$2360)                                                           001177
00707    249*           IF (LN.LE.0.OR.LN.GT.NASH) GO TO 2360                                             001204
00711    250*           IF (KOUT.EQ.1) GO TO 2366                                                         001221
00711    251*      C    DELETE                                                                            001221
00713    252*           L1=LN+1                                                                           001224
00714    253*           IF (LN.EQ.NASH) GO TO 2364                                                        001227
00716    254*           DO 2362 I=L1,NASH                                                                 001234
00721    255*           DO 2362 J=1,11                                                                    001245
00724    256*           ACOMP(J,I-1)=ACOMP(J,I)                                                           001245
00725    257*      2362 CONTINUE                                                                          001250
00730    258*      2364 NASH=NASH-1                                                                       001250
00731    259*           GO TO 2352                                                                        001252
00731    260*      C    ALTER                                                                             001252
00732    261*      2366 NI=LN                                                                             001254
00733    262*           GO TO 2372                                                                        001255
00733    263*      C    ADD                                                                               001255
00734    264*      2370 NASH=NASH+1                                                                       001257
00735    265*           NI=NASH                                                                           001261
00735    266*      C    READ IN NEW DATA                                                                  001261
00736    267*      2372 CALL GOUT(' LBS/100 LBS DRY ASH AND COMPONENT',34)                                001263
00737    268*           DO 2374 J=1,5                                                                     001266
00742    269*           IACOMP(J*2,NI)=2H                                                                 001300
00743    270*      2374 ACOMP(J*2+1,NI)=0.                                                                001301
00745    271*           CALL RDATAF(11,ACOMP(1,NI),$2372)                                                 001303
00746    272*           GO TO 2352                                                                        001313
00746    273*      C    CHECK FOR FES2                                                                    001313
00747    274*      2380 FES2=0.                                                                           001315
00750    275*           DO 2386 I=1,NASH                                                                  001315
00753    276*           DO 2384 J=1,5                                                                     001334
00756    277*           IF (IACOMP(J*2,I).NE.IASH(J*2-1,4)) GO TO 2386                                    001334
00760    278*           IF (ACOMP(J*2+1,I).NE.ASH(J*2,4)) GO TO 2386                                      001337
00762    279*      2384 CONTINUE                                                                          001346
00764    280*           FES2=ACOMP(1,I)                                                                   001346
00765    281*           GO TO 380                                                                         001350
00766    282*      2386 CONTINUE                                                                          001354
00770    283*           GO TO 380                                                                         001354
00771    284*       351 CONTINUE                                                                          001356
00771    285*      C    READ IN ASH COMPONENTS                                                            001356
00772    286*           CALL GOUT(' TYPE LBS/100 LBS DRY ASH FOR COMPONENTS',40)                          001356
00773    287*           CALL GOUT(' STATE ASSUMED SOLID. COAL TEMPERATURE ASSUMED.',47)                   001361
00774    288*       352 CALL GOUT(' SIO2',5)                                                              001366
00775    289*           CALL RDATAF(1,ACOMP(1,1),$352)                                                    001371
00776    290*       354 CALL GOUT(' FE2O3',6)                                                             001377
00777    291*           CALL RDATAF(1,ACOMP(1,2),$354)                                                    001402
01000    292*       356 CALL GOUT(' AL2O3',6)                                                             001410
01001    293*           CALL RDATAF(1,ACOMP(1,3),$356)                                                    001413
01002    294*       358 CALL GOUT(' FES2',5)                                                              001421
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01003                 CALL RDATAF(1,ACOMP(1,4),$358)                                001424
01004                 FES2=ACOMP(1,4)                                               001431
01005                 IF (IACOMP(1,4).EQ.'      ') FES2=0.                          001433
01007                 J=0                                                           001437
01007         C       REMOVE ANY ZERO COMPONENTS                                    001437
01010                 DO 364 I=1,4                                                  001444
01013                 IF (ACOMP(1,I)) ,364,                                         001450
01016                 IF (IACOMP(1,I).EQ.'      ') GO TO 364                        001452
01020                 J=J+1                                                         001455
01021                 ACOMP(1,J)=ACOMP(1,I)                                         001461
01022                 IF (I.NE.J) ACOMP(1,I)=0.                                     001462
01024                 DO 362 LL=1,10                                                001466
01027             362 ACOMP(LL+1,J)=ASH(LL,I)                                       001477
01031             364 CONTINUE                                                      001504
01033                 NI=J+1                                                        001504
01033         C       ADD OTHER ASH COMPONENTS                                      001504
01034                 CALL GOUT(' CONTINUE WITH ASH COMPONENTS',29)                 001507
01035                 CALL GOUT(' LBS/100 LBS DRY ASH AND COMPONENT',34)            001513
01036             366 CALL GOUT('     EXAMPLE  0.25  2HTI  1.  1HO  2.',38)         001520
01037             367 DO 368 J=1,5                                                  001524
01042                 IACOMP(J*2,NI)=2H                                             001535
01043             368 ACOMP(J*2+1,NI)=0.                                            001536
01045             370 CALL RDATAF(11,ACOMP(1,NI),$366)                              001540
01046                 IF (ACOMP(1,NI)) ,372,                                        001550
01051                 IF (IACOMP(1,NI).EQ.'      ') GO TO 372                       001552
01053                 NI=NI+1                                                       001555
01054                 GO TO 367                                                     001560
01055             372 NASH=NI-1                                                     001562
01056             380 IF (JOPT(5).EQ.0) GO TO 390                                   001565
01056         C       READ COAL CONVERSION FRACTION                                 001565
01060             382 CALL GOUT(' TYPE CARBON CONVERSION FRACTION, FOR EXAMPLE, 0.89',   001567
01060                X   51)                                                        001567
01061                 CALL RDATAF(1,PER,$382)                                       001572
01061         C       COMPUTE VALUES FOR HHV BY DIFFERENT FORMULAS                  001572
01062             390 CONTINUE                                                      001600
01063                 HH(2)=145.44*COAL(1,2)+620.28*(COAL(2,2)-0.125*COAL(4,2))     001600
01063                X  +40.50*COAL(5,2)                                            001600
01064                 HH(3)=146.0*COAL(1,2)+620.0*(COAL(2,2)-0.125*COAL(4,2))       001614
01064                X  +40.50*COAL(5,2)                                            001614
01065                 HH(4)=144.9*COAL(1,2)+610.0*(COAL(2,2)-0.125*COAL(4,2))       001623
01065                X    +55.50*COAL(5,2)                                          001623
01066                 HH(5)=(654.3*COAL(2,2)/(100.-PROX(3))+424.62)*                001634
01066                X    (COAL(1,2)/3.+COAL(2,2)-0.125*(COAL(4,2)-COAL(5,2)))      001634
01067                 HH(6)=146.58*COAL(1,2)+568.78*COAL(2,2)+29.4*COAL(5,2)        001653
01067                X    -6.58*PROX(3)-51.53*(COAL(3,2)+COAL(4,2))                 001653
01070                 HH(7)=AMAX1(HH(2),HH(3),HH(4),HH(5),HH(6))                    001673
01071                 HH(8)=AMIN1(HH(2),HH(3),HH(4),HH(5),HH(6))                    001715
01072                 DO 392 I=2,8                                                  001743
01075                 ENCODE (394,HHT(I*5-1)) HH(I)                                 001743
01100             392 CONTINUE                                                      001753
01102             394 FORMAT (F12.3)                                                001753
01103                 IF (JOPT(7).EQ.0) GO TO 420                                   001753
01105                 CALL GOUT(' HHV CALCULATION',16)                              001755
01106                 DO 398 I=1,8                                                  001764
01111                 CALL GOUT(HHT(I*5-4),30)                                      001764
01112             398 CONTINUE                                                      001773
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 01114     351*        400 CALL RDATAI(1,IE,$400)                                                 001773
 01115     352*            IF (IE.LT.0.OR.IE.GT.8) GO TO 400                                      001777
 01117     353*            IF (IE.GT.0) GO TO 420                                                 002014
 01121     354*        402 CALL GOUT(' ENTER HHV AS BTU/LB COAL',25)                              002020
 01122     355*            CALL RDATAF(1,HH(1),$402)                                              002023
 01123     356*        420 HHVV=HH(IE+1)                                                          002031
 01124     357*            IF (JOPT(8).EQ.0) GO TO 440                                            002033
 01126     358*            IF (IOPT.NE.1) GO TO 421                                               002035
 01130     359*            ENCODE (2350,IOUT) JOPT(8)                                             002040
 01133     360*            CALL GOUT(IOUT,18)                                                     002046
 01134     361*       2420 IF (NFUEL.EQ.0) GO TO 2427                                             002053
 01136     362*            DO 2426 I=1,NFUEL                                                      002054
 01141     363*            ENCODE (2424,IOUT) I,OFUEL(1,I),OFUEL(2,I),IOFUEL(3,I),                002063
 01141     364*          X    (IOFUEL(J*2+2,I),OFUEL(J*2+3,I),J=1,5)                              002063
 01154     365*       2424 FORMAT (I4,F10.4,F10.3,1X,A3,5(2X,A2,2X,F8.4))                         002101
 01155     366*            CALL GOUT(IOUT,98)                                                     002101
 01156     367*       2426 CONTINUE                                                               002112
 01160     368*       2427 CALL GOUT(' TYPE 1-ALTER, 2-DELETE, 3-ADD, RETURN TO CONTINUE',50)     002112
 01161     369*       2422 KOUT=0                                                                 002116
 01162     370*            CALL RDATAI(1,KOUT,$2422)                                              002116
 01163     371*            IF (KOUT.LT.0.OR.KOUT.GT.3) GO TO 2422                                 002123
 01165     372*            IF (KOUT.EQ.0) GO TO 430                                               002140
 01167     373*            IF (KOUT.EQ.3) GO TO 2434                                              002142
 01171     374*            CALL GOUT(' TYPE LINE NUMBER',17)                                      002145
 01172     375*       2428 LN=0                                                                   002152
 01173     376*            CALL RDATAI(1,LN,$2428)                                                002152
 01174     377*            IF  (LN.LE.0.OR.LN.GT.NFUEL) GO TO 2428                                002157
 01176     378*            IF (KOUT.EQ.1) GO TO 2432                                              002174
 01176     379*      C     DELETE                                                                 002174
 01200     380*            L1=LN+1                                                                002177
 01201     381*            IF (LN.EQ.NFUEL) GO TO 2431                                            002202
 01203     382*            DO 2430 I=1,NFUEL                                                      002205
 01206     383*            DO 2430 J=1,13                                                         002213
 01211     384*            OFUEL(J,I-1)=OFUEL(J,I)                                                002213
 01212     385*       2430 CONTINUE                                                               002216
 01215     386*       2431 NFUEL=NFUEL-1                                                          002216
 01216     387*            GO TO 2420                                                             002220
 01216     388*      C     ALTER                                                                  002220
 01217     389*       2432 NI=LN                                                                  002222
 01220     390*            GO TO 2436                                                             002223
 01220     391*      C     ADD                                                                    002223
 01221     392*       2434 NFUEL=NFUEL+1                                                          002225
 01222     393*            NI=NFUEL                                                               002227
 01222     394*      C     READ IN NEW DATA                                                       002227
 01223     395*       2436 CALL GOUT(' TYPE LBS/LB COAL, TEMPERATURE (DEG F) AND STATE AND CO     002231
 01223     396*           XMPONENT',63)                                                           002231
 01224     397*            DO 2438 I=1,5                                                          002234
 01227     398*            IOFUEL(J*2+2,NI)=2H                                                    002246
 01230     399*       2438 OFUEL(J*2+3,NI)=0.                                                     002247
 01232     400*            OFUEL(1,NI)=0.                                                         002251
 01233     401*            OFUEL(2,NI)=0.                                                         002253
 01234     402*            IOFUEL(3,NI)='      '                                                  002254
 01235     403*            CALL RDATAF(13,OFUEL(1,NI),$2436)                                      002256
 01236     404*            GO TO 2420                                                             002265
 01237     405*        421 CONTINUE                                                               002267
 01237     406*      C     READ IN OTHER FUEL COMPONENTS                                          002267
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01240   407.          CALL GOUT(' TYPE OTHER FUEL COMPONENTS',27)                  002267
01241   408.          CALL GOUT(' TYPE LBS/LB COAL, TEMPERATURE (DEG F) AND STATE AND CO   002272
01241   409.         XMPONENT',63)                                                  002272
01242   410.          NI=1                                                         002276
01243   411.      422 CALL GOUT('      EXAMPLE  0.31  100.  1HG  1HH  2.  1HO  1.',47)   002301
01244   412.      423 DO 424 J=1,5                                                 002305
01247   413.          IOFUEL(J*2-2,NI)=2H                                          002316
01250   414.      424 OFUEL(J*2-3,NI)=0.                                           002317
01252   415.          OFUEL(1,NI)=0.                                               002321
01253   416.          OFUEL(2,NI)=0.                                               002323
01254   417.          IOFUEL(3,NI)='        '                                      002324
01255   418.      426 CALL RDATAF(13,OFUEL(1,NI),$422)                             002326
01256   419.          IF (OFUEL(1,NI)) ,428,                                       002335
01261   420.          IF (IOFUEL(1,NI).EQ.'        ') GO TO 428                    002337
01263   421.          NI=NI+1                                                      002342
01264   422.          GO TO 423                                                    002345
01265   423.      428 NFUEL=NI-1                                                   002347
01266   424.      430 WCR=0.                                                       002362
01267   425.          DO 434 I=1,NFUEL                                             002352
01272   426.          DO 432 J=1,5                                                 002370
01275   427.          IF (IOFUEL(J*2-2,I).NE.IH2O(J)) GO TO 434                    002370
01277   428.          IF (OFUEL(J*2-3,I).NE.H2O(J)) GO TO 434                      002373
01301   429.      432 CONTINUE                                                     002401
01303   430.          WCR=OFUEL(1,I)                                               002401
01304   431.          GO TO 440                                                    002403
01305   432.      434 CONTINUE                                                     002410
01307   433.      440 IF (JOPT(9).EQ.0) GO TO 450                                  002410
01307   434.    C     READ IN OXIDIZER TEMPERATURE                                 002410
01311   435.      442 CALL GOUT(' TYPE IN OXIDIZER TEMPERATURE, DEG F',36)         002412
01312   436.          CALL RDATAF(1,OTEMP,$442)                                    002415
01313   437.      450 IF (JOPT(10).EQ.0) GO TO 470                                 002423
01313   438.    C     READ IN OXIDIZER COMPONENTS                                  002423
01315   439.          CALL GOUT(' TYPE OXIDIZER COMPONENTS',25)                    002426
01316   440.          CALL GOUT(' TYPE LBS/100 LBS OXIDIZER AND COMPONENT',40)     002430
01317   441.          NI=1                                                         002434
01320   442.      452 CALL GOUT('      EXAMPLE  95.0  1HO  2.',27)                 002437
01321   443.      453 DO 454 J=1,5                                                 002443
01324   444.          IOXID(J*2,NI)=2H                                             002454
01325   445.      454 OXID(J*2-1,NI)=0.                                            002455
01327   446.      456 CALL RDATAF(11,OXID(1,NI),$452)                              002457
01330   447.          IF (OXID(1,NI)) ,460,                                        002467
01333   448.          IF (IOXID(1,NI).EQ.'        ') GO TO 460                     002471
01335   449.          NI=NI+1                                                      002474
01336   450.          GO TO 453                                                    002477
01337   451.      460 NOXID=NI-1                                                   002501
01340   452.      470 CONTINUE                                                     002504
01340   453.    C     COMPUTATION FOR COAL CARD                                    002504
01341   454.          SINRT=COAL(1,2)*(1.-PER)                                     002504
01342   455.          COAL(1,2)=COAL(1,2)*PER                                      002507
01343   456.          SUM=0.                                                       002512
01344   457.          N=NREAC+1                                                    002513
01345   458.          NS=N                                                         002516
01346   459.          DO 482 I=1,5                                                 002531
01351   460.      482 SUM=SUM+COAL(I,2)                                            002531
01353   461.          DO 484 I=1,5                                                 002541
01356   462.      484 ANUM(N,I)=(COAL(I,2)/SUM)*100.                               002541
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01360     463.              SUM1=0.                                                         002545
01361     464.              DO 486 I=1,5                                                    002553
01364     465.              ANUM(N,I)=ANUM(N,I)/PMOL(I)                                     002553
01365     466.          486 SUM1=SUM1+ANUM(N,I)                                             002555
01367     467.              DO 488 I=1,5                                                    002565
01372     468.          488 ANUM(N,I)=(ANUM(N,I)/SUM1)*100.                                 002565
01372     469.        C     CREATE COAL CARD                                                002565
01374     470.              DO 494 I=1,5                                                    002576
01377     471.          494 NAME(N,I)=ICOAL(I,1)                                            002576
01401     472.              NAME(N,6)=1H                                                    002600
01402     473.              ANUM(N,6)=0.                                                    002602
01402     474.        C     COMPUTE COAL/FUEL RATIO                                         002602
01403     475.              CSUM=0.                                                         002603
01404     476.              DO 498 I=1,NFUEL                                                002607
01407     477.          498 CSUM=CSUM+OFUEL(1,I)                                            002607
01411     478.              CF=1.0/(1.0+CSUM)                                               002612
01412     479.              PECWT(N)=CF*SUM/100.                                            002616
01413     480.              MOLE(N)=1H                                                      002621
01414     481.              FAZ(N)=1HS                                                      002623
01415     482.              RTEMP(N)=(CTEMP-32.)/1.8+273.15                                 002625
01416     483.              FOX(N)=1HF                                                      002632
01417     484.              DENS(N)=0.                                                      002634
01420     485.              NREAC=NREAC+1                                                   002635
01420     486.        C     CREATE INERT CARBON CARD                                        002635
01421     487.              IF (PER-1.) ,504,                                               002640
01424     488.              N=NREAC+1                                                       002643
01425     489.              DO 500 I=1,6                                                    002645
01430     490.              NAME(N,I)=4H                                                    002653
01431     491.          500 ANUM(N,2)=0.                                                    002654
01433     492.              NAME(N,1)='IC   '                                               002656
01434     493.              ANUM(N,1)=1.                                                    002660
01435     494.              PECWT(N)=CF*SINRT/100.                                          002662
01436     495.              MOLE(N)=1H                                                      002666
01437     496.              ENTH(N)=0.                                                      002667
01440     497.              NAME(N,6)=2H00                                                  002670
01441     498.              FAZ(N)=1HS                                                      002672
01442     499.              RTEMP(N)=RTEMP(NS)                                              002674
01443     500.              FOX(N)=1HF                                                      002677
01444     501.              DENS(N)=0.                                                      002701
01445     502.              NREAC=NREAC+1                                                   002702
01445     503.        C     CREATE OTHER COAL COMPONENTS CARDS                              002702
01446     504.          504 IF (NCOAL.EQ.0) GO TO 520                                       002706
01450     505.              N=NREAC                                                         002707
01451     506.              DO 508 I=1,NCOAL                                                002715
01454     507.              DO 506 J=1,5                                                    002734
01457     508.              NAME(N+I,J)=ICCOMP(J*2+1,I)                                     002734
01460     509.          506 ANUM(N+I,J)=CCOMP(J*2+2,I)                                      002735
01462     510.              PECWT(N+I)=CCOMP(1,I)*CF/100.                                   002740
01463     511.              MOLE(N+I)=1H                                                    002744
01464     512.              IFAZ(N+I)=ICCOMP(2,I)                                           002746
01465     513.              ENTH(N+I)=0.                                                    002750
01466     514.              NAME(N+I,6)=2H00                                                002751
01467     515.              ANUM(N+I,6)=0.                                                  002753
01470     516.              RTEMP(N+I)=(CTEMP-32.)/1.8+273.15                               002754
01471     517.              FOX(N+I)=1HF                                                    002756
01472     518.              DENS(N+I)=0.                                                    002760
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01473     519*        508 CONTINUE                                                                     002767
01475     520*        520 NREAC=NREAC+NCOAL                                                            002767
01475     521*    C       CREATE CARDS FOR ASH COMPONENTS                                              002767
01476     522*            N=NREAC                                                                      002771
01477     523*            SUM2=0.                                                                      002772
01500     524*            IF (NASH.EQ.0) GO TO 540                                                     002773
01502     525*            ASHF=CF*PROX(3)/100.                                                         002775
01503     526*            DO 522 I=1,NASH                                                              003010
01506     527*        522 SUM2=SUM2+ACOMP(1,I)                                                         003021
01510     528*            DO 528 I=1,NASH                                                              003035
01513     529*            DO 526 J=1,5                                                                 003035
01516     530*            NAME(N+I,J)=IACOMP(J*2,I)                                                    003036
01517     531*        526 ANUM(N+I,J)=ACOMP(J*2+1,I)                                                   003036
01521     532*            PECWT(N+I)=(ACOMP(1,I)*ASHF)/SUM2                                            003041
01522     533*            MOLE(N+I)=1H                                                                 003045
01523     534*            FAZ(N+I)=1HS                                                                 003047
01524     535*            ENTH(N+I)=0.                                                                 003051
01525     536*            NAME(N+I,6)=2H00                                                             003052
01526     537*            ANUM(N+I,6)=0.                                                               003054
01527     538*            RTEMP(N+I)=(CTEMP-32.)/1.8+273.15                                            003055
01530     539*            FOX(N+I)=1HF                                                                 003057
01531     540*            DENS(N+I)=0.                                                                 003061
01532     541*        528 CONTINUE                                                                     003070
01534     542*        540 NREAC=NREAC+NASH                                                             003070
01534     543*    C       COMPUTE ENTHALPY FOR COAL                                                    003070
01535     544*            FES2=FES2*ASHF/(SUM2*CF)                                                     003072
01536     545*            HHV=((HHVV-14485.7*SINRT/100.)/1.8)*(100./SUM)*(100./SUM1)*100.              003100
01537     546*            FES2C=(100./(1.8*119.85))*(100./SUM)*(100./SUM1)*FES2                        003117
01540     547*            HF1=-ANUM(NS,1)*94051.8-0.5*ANUM(NS,2)*68317.4                               003124
01540     548*        X      -ANUM(NS,5)*70960.-FES2C*197650.                                          003124
01541     549*            PX=100.*PROX(1)/(PROX(1)+PROX(2))                                            003141
01542     550*            HF2=(.175*(CTEMP-77)+.0029*PX*(CTEMP-77)+                                    003147
01542     551*        X      0.00025*(CTEMP-60)**2-0.07225)*(100./SUM1)*(100./1.8)                     003147
01543     552*            ENTH(NS)=HHV+HF1+HF2                                                         003167
01543     553*    C       CREATE CARDS FOR OTHER FUEL COMPONENTS                                       003167
01544     554*            N=NREAC                                                                      003172
01545     555*            IF (NFUEL.EQ.0) GO TO 560                                                    003173
01547     556*            DO 548 I=1,NFUEL                                                             003200
01552     557*            DO 546 J=1,5                                                                 003214
01555     558*            NAME(N+I,J)=IOFUEL(J*2+2,I)                                                  003214
01556     559*        546 ANUM(N+I,J)=OFUEL(J*2+3,I)                                                   003215
01560     560*            PECWT(N+I)=OFUEL(1,I)*CF                                                     003220
01561     561*            MOLE(N+I)=1H                                                                 003223
01562     562*            IFAZ(N+I)=IOFUEL(3,I)                                                        003225
01563     563*            ENTH(N+I)=0.                                                                 003227
01564     564*            NAME(N+I,6)=2H00                                                             003230
01565     565*            ANUM(N+I,6)=0.                                                               003232
01566     566*            RTEMP(N+I)=(OFUEL(2,I)-32.)/1.8+273.15                                       003233
01567     567*            FOX(N+I)=1HF                                                                 003240
01570     568*            DENS(N+I)=0.                                                                 003242
01571     569*        548 CONTINUE                                                                     003253
01571     570*    C       LOOK UP CARBON                                                               003253
01573     571*            DO 552 I=1,NFUEL                                                             003253
01576     572*            DO 550 J=1,5                                                                 003263
01601     573*            IF (NAME(N+I,J).NE.ICC(J)) GO TO 552                                         003263
01603     574*            IF (ANUM(N+I,J)-CC(J)) 552,,552                                              003266
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ORIGINAL PAGE IS
OF POOR QUALITY

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 01606     575*      550 CONTINUE                                                                 003274
 01610     576*          GO TO 554                                                                003274
 01611     577*      552 CONTINUE                                                                 003277
 01613     578*          GO TO 560                                                                003277
 01613     579*   C      CREATE INERT CARBON CARD FOR RECYCLE CARBON                              003277
 01615     580*      554 DO 556 J=1,6                                                             003301
 01617     581*          NAME(N+NFUEL+1,J)=NAME(N+I,J)                                            003322
 01620     582*      556 ANUM(N+NFUEL+1,J)=ANUM(N+I,J)                                            003323
 01622     583*          NAME(N+NFUEL+1,1)=.IC  .                                                 003326
 01623     584*          PECWT(N+NFUEL+1)=(1.-PER)*PECWT(N+I)                                     003331
 01624     585*          PECWT(N+I)=PER*PECWT(N+I)                                                003336
 01625     586*          MOLE(N+NFUEL+1)=MOLE(N+I)                                                003341
 01626     587*          FAZ(N+NFUEL+1)=FAZ(N+I)                                                  003343
 01627     588*          ENTH(N+NFUEL+1)=ENTH(N+I)                                                003345
 01630     589*          RTEMP(N+NFUEL+1)=RTEMP(N+I)                                              003347
 01631     590*          FOX(N+NFUEL+1)=FOX(N+I)                                                  003351
 01632     591*          DENS(N+NFUEL+1)=DENS(N+I)                                                003353
 01633     592*          NREAC=NREAC+1                                                            003355
 01634     593*      560 NREAC=NREAC+NFUEL                                                        003361
 01634     594*   C      CREATE CARDS FOR OXIDIZER COMPONENTS                                     003361
 01635     595*          N=NREAC                                                                  003363
 01636     596*          IF (NOXID.EQ.0) GO TO 590                                                003364
 01640     597*          SUM3=0.                                                                  003366
 01641     598*          DO 572 I=1,NOXID                                                         003376
 01644     599*      572 SUM3=SUM3+OXID(1,I)                                                      003407
 01646     600*          DO 578 I=1,NOXID                                                         003423
 01651     601*          DO 576 J=1,5                                                             003423
 01654     602*          NAME(N+I,J)=IOXID(J*2,I)                                                 003423
 01655     603*      576 ANUM(N+I,J)=OXID(J*2+1,I)                                                003424
 01657     604*          PECWT(N+I)=OXID(1,I)/SUM3                                                003427
 01660     605*          MOLE(N+I)=1H                                                             003432
 01661     606*          FAZ(N+I)=1HG                                                             003434
 01662     607*          ENTH(N+I)=0.                                                             003436
 01663     608*          NAME(N+I,6)=2H00                                                         003437
 01664     609*          ANUM(N+I,6)=0.                                                           003441
 01665     610*          RTEMP(N+I)=(OTEMP-32.)/1.8+273.15                                        003442
 01666     611*          FOX(N+I)=1HO                                                             003444
 01667     612*          DENS(N+I)=0.                                                             003446
 01670     613*      578 CONTINUE                                                                 003455
 01672     614*      590 NREAC=NREAC+NOXID                                                        003455
 01672     615*   C      SAVE COAL DATA                                                           003455
 01673     616*          COAL(1,2)=COAL(1,2)/PER                                                  003457
 01674     617*          REWIND IC                                                                003462
 01675     618*          WRITE (IC) NREAC,CF,HHVY,WCR,PER                                         003465
 01704     619*          WRITE (IC) CTEMP,OTEMP                                                   003476
 01710     620*          WRITE (IC) PROX,COAL,PER,IE,HH                                           003504
 01717     621*          WRITE (IC) NCOAL,NASH,NFUEL,NOXID                                        003524
 01725     622*          WRITE (IC) ((CCOMP(I,J),I=1,12),J=1,NCOAL),                              003552
 01725     623*         X   ((ACOMP(I,J),I=1,11),J=1,NASH),                                       003552
 01725     624*         X   ((OFUEL(I,J),I=1,13),J=1,NFUEL),                                      003552
 01725     625*         X   ((OXID(I,J),I=1,11),J=1,NOXID)                                        003552
 01725     626*   C      WRITE OUT REACTANT FILE                                                  003552
 01763     627*          WRITE (IC) NREAC,CF                                                      003606
 01767     628*          DO 610 I=1,NREAC                                                         003620
 01772     629*          WRITE (IC) (NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),                 003620
 01772     630*         X   ENTH(I),NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOX(I),DENS(I)            003620
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  02012     631*       610 CONTINUE                                                          003646
  02014     632*           ENDFILE IC                                                        003646
  02015     633*       680 CONTINUE                                                          003652
  02016     634*           RETURN                                                            003652
  02017     635*           END                                                               003712

        END OF COMPILATION:          NO  DIAGNOSTICS.

  @HDG,P       CPHS
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@FOR,S      CPHS,CPHS
HSA  E3 -10/15/80-13:06:13 (11,)

  SUBROUTINE CPHS        ENTRY POINT 000567

  STORAGE USED: CODE(1) 000603; DATA(0) 000160; BLANK COMMON(2) 000000

   COMMON BLOCKS:

   0003     SPECES  017106
   0004     MISC    001701
   0005     INDX    000041
   0006     LOWTH   001201
   0007     CCC     000003

  EXTERNAL REFERENCES (BLOCK, NAME)

   0010     NWDU$
   0011     NI02$
   0012     ALOG
   0013     NI01$
   0014     NERR3$

  STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

   0001     000031 10L        0001     000207 171G       0001     000217 174G       0001     000043 20L        0001     000351 221G
   0001     000462 254G       0001     000065 30L        0001     000067 31L        0001     000157 32L        0000     000041 3333F
   0001     000164 40L        0001     000176 60L        0001     000230 70L        0001     000233 80L        0001     000412 87L
   0000     000060 88F        0001     000472 89L        0001     000531 90L        0000     000103 904F       0003     011052 A
   0004     000640 AM         0004     000705 AM1        0004     001135 ANUM       0004     000004 ATOM       0004     000514 BO
   0004     000545 BOP        0005     000036 CALCH      0003 R   000000 COEF       0005     000001 CONVG      0006 R   000361 CPL
   0004     000706 CPR1       0004 R   000634 CPSUM      0000 R   000040 CPUSED     0000 R   000035 CPX        0000 R   000007 CPXY
   0004     000654 DATA       0003     010624 DELN       0007     000002 DEMAND     0004     001560 DENS       0003 R   004312 EN
   0003     010150 ENLN       0004     001700 ENLSAV     0004     000000 ENN        0004     001676 ENNL       0004     001677 ENSAVE
   0004     001414 ENTH       0004     000636 EQRAT      0004     001445 FAZ        0004     001527 FOX        0007     000000 GRAPH
   0006 R   000551 HL         0005     000003 HP         0004     000642 HPP        0004     000637 HSUBO      0000 R   000034 HX
   0000 R   000013 HXX        0003 R   010376 HO         0000 I   000037 I          0005     000030 IC         0005     000000 IDEBUG
   0000 I   000001 IER        0000 I   000023 IEXTND     0006 I   001131 ILSP       0005     000015 IMAT       0000 I   000002 IMSG
   0005     000132 INJPS      0005     000023 IONS       0005     000021 IP         0005     000037 IOSAVE     0005     000016 IO1
   0005     000005 ISV        0005     000034 IT         0003 I   016266 IUSE       0000 I   000026 IX         0005 I   000031 J
   0005     000026 JLIQ       0007 I   000001 JOUT       0005     000025 JSOL       0000 I   000024 K          0000 I   000025 KK
   0005     000014 KMAT       0000 I   000027 KX         0004     000463 LLMT       0005     000040 LSAVE      0000 I   000036 M
   0005     000006 MOLES      0004     000707 NAME       0005     000024 NC         0005     000022 NEWR       0005     000035 NFZ
   0005     000012 NLM        0006 I   000000 NLTSP      0005     000017 NOF        0005     000020 NOMIT      0005     000007 NP
   0005 I   000011 NPT        0005     000027 NREAC      0005 I   000013 NS         0000 I   000000 NSPP1      0005     000010 NT
   0000 I   000030 NTUP       0004     000635 OF         0004     001644 OXF        0004     001363 PECWT      0004     000633 PP
   0004     000644 RH         0004     001611 RHOP       0004     001612 RMW        0004     001476 RTEMP      0003 R   004064 S
   0005     000033 SHOCK      0006 R   000741 SL         0003     016660 SLN        0005     000004 SP         0003 I   015364 SUB
   0006 I   000001 SUBLT      0004     000001 SUMN       0000 R   000033 SX         0000 R   000017 SXX        0004     000003 SO
   0003     016514 TEMP       0004     000632 THIGH      0006 R   000171 TL         0004 R   001643 TLN        0000 R   000032 TLNS
   0004 R   000630 TLOW       0004     000627 TM         0004 R   000631 TMID       0005     000002 TP         0004 R   000002 TT
   0000 R   000031 TTS        0000 R   000003 TXX        0004     000646 VMIN       0005     000032 VOL        0004     000650 VPLS
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 0004   000652 WP

 00101      1*             SUBROUTINE CPHS                                                              000002
 00101      2*       C                                                                                  000002
 00101      3*       C     CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES                   000002
 00101      4*       C                                                                                  000002
 00101      5*       C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)              000002
 00101      6*       C     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)              000002
 00103      7*             INCLUDE SPECPK                                                               000002
 00107      8*             COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                    000002
 00107      9*            1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                000002
 00107     10*            2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),       /MISC/   000002
 00107     11*            3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),              000002
 00107     12*            4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,              000002
 00107     13*            5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                         000002
 00110     14*             COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,       /INDX/   000002
 00110     15*            1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,     /INDX/   000002
 00110     16*            2              NREAC,IC,J,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE         /INDX/   000002
 00111     17*             COMMON /LOWTH/ NLTSP,SUBLT(40,3),TL(40,3),CPL(40,3),HL(40,3),       /LOWTH/  000002
 00111     18*            1                SL(40,3),ILSP(40)                                   /LOWTH/  000002
 00111     19*       C                                                                                  000002
 00112     20*                COMMON /CCC/ GRAPH,JOUT,DEMAND                                            000002
 00112     21*       C                                                                                  000002
 00113     22*             DATA IER/0/,IMSG/-1/                                                         000002
 00116     23*             DIMENSION TXX(4),CPXX(4),HXX(4),SXX(4)                           CPHS  20   000002
 00117     24*             INTEGER SUB,SUBLT                                                            000002
 00117     25*       C                                                                                  000002
 00120     26*             IEXTND = 0                                                       CPHS 190   000002
 00121     27*             IF(TT.LT.TLOW) IEXTND = 1                                        CPHS 200   000003
 00123     28*             IF(IEXTND.NE.0) IMSG = IMSG + 1                                  R FEB-3    000011
 00125     29*             IF(IMSG.NE.0) GO TO 10                                           R FEB-3    000016
 00127     30*             IF(IEXTND.NE.0) WRITE(JOUT,3333) TT                                         000020
 00133     31*       3333  FORMAT (//25X,48HLOW TEMPERATURE THERMO EXTENSION IN CPHS AT TT =,          000031
 00133     32*            1         F12.6,15H DEGREES KELVIN//)                                        000031
 00134     33*         10  K = 1                                                                       000031
 00135     34*             IF (TT.LE.TMID) K=2                                              CPHS 240   000032
 00137     35*             KK=0                                                             CPHS 250   000040
 00140     36*             CPSUM=0.                                                         CPHS 260   000041
 00141     37*       20    IF (COEF(K,1,J).NE.0.) GO TO 30                                  CPHS 270   000043
 00143     38*             IF (IUSE(J).LT.0) GO TO 40                                       CPHS 280   000047
 00145     39*             KK=K                                                             CPHS 290   000053
 00146     40*             K=1                                                              CPHS 300   000055
 00147     41*             IF (KK.EQ.1) K=2                                                 CPHS 310   000057
 00151     42*         30  IF (IEXTND .NE. 0)  GO TO 60                                                000065
 00153     43*         31  S(J) = ((((COEF(K,5,J)/4.0)*TT + COEF(K,4,J)/3.0)*TT + COEF(K,3,J)          000067
 00153     44*            1       /2.0)*TT + COEF(K,2,J))*TT + COEF(K,1,J)*TLN + COEF(K,7,J)          000067
 00154     45*             HO(J)=((((COEF(K,5,J)/5.)*TT+COEF(K,4,J)/4.)*TT+COEF(K,3,J)/3.)*TTCPHS 370   000114
 00154     46*            1+COEF(K,2,J)/2.)*TT+COEF(K,1,J)+COEF(K,6,J)/TT                   CPHS 380   000114
 00155     47*             CPSUM=CPSUM+((((COEF(K,5,J)*TT+COEF(K,4,J))*TT+COEF(K,3,J))*TT+COECPHS 390   000140
 00155     48*            1F(K,2,J))*TT+COEF(K,1,J))*EN(J,NPT)                              CPHS 400   000140
 00156     49*         32  IF (KK .EQ. 0)  GO TO 40                                                    000157
 00160     50*             K=KK                                                             CPHS 430   000160
 00161     51*             KK=0                                                             CPHS 440   000162
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00162     52*      40   IF (J .EQ. NS)  RETURN                                                          000164
00164     53*           J=J+1                                                             CPHS 460      000171
00165     54*           GO TO 20                                                          CPHS 470      000174
00166     55*      60   IF (NLTSP .EQ. 0)  GO TO 31                                                     000176
00170     56*           DO 70 IX= 1,NLTSP                                                 CPHS 500      000177
00173     57*           DO 65 KX = 1,3                                                                  000217
00176     58*      65   IF (SUB(J,KX) .NE. SUBLT(IX,KX))  GO TO 70                                      000217
00201     59*           GO TO 80                                                          CPHS 540      000226
00202     60*      70   CONTINUE                                                          CPHS 550      000231
00204     61*           GO TO 31                                                          CPHS 560      000231
00205     62*      80   NTUP = ILSP(IX)                                                                 000233
00206     63*           IF(TT.LT.TL(IX,1)) GO TO 90                                       CPHS 590      000236
00210     64*           TTS = TT                                                          CPHS 600      000241
00211     65*           TLNS= TLN                                                         CPHS 610      000243
00212     66*           TT = TLOW                                                         CPHS 620      000245
00213     67*           TLN= ALOG(TT)                                                     CPHS 630      000247
00214     68*           KX = 2                                                            CPHS 640      000253
00215     69*           SX =((((COEF(KX,5,J)/4.)*TT+COEF(KX,4,J)/3.)*TT+COEF(KX,3,J)/2.)  CPHS 650      000255
00215     70*          1     *TT+COEF(KX,2,J))*TT+COEF(KX,1,J)*TLN+COEF(KX,7,J)           CPHS 660      000255
00216     71*           HX =((((COEF(KX,5,J)/5.)*TT+COEF(KX,4,J)/4.)*TT+COEF(KX,3,J)/3.)  CPHS 670      000301
00216     72*          1     *TT+COEF(KX,2,J)/2.)*TT+COEF(KX,1,J)+COEF(KX,6,J)/TT         CPHS 680      000301
00217     73*           CPX=(((COEF(KX,5,J)*TT+COEF(KX,4,J))*TT+COEF(KX,3,J))*TT          CPHS 690      000325
00217     74*          1     +COEF(KX,2,J))*TT+COEF(KX,1,J)                               CPHS 700      000325
00220     75*           DO 86 KX = 1,NTUP                                                               000351
00223     76*           TXX(KX) = TL(IX,KX)                                                             000351
00224     77*           CPXX(KX) = CPL(IX,KX)                                                           000352
00225     78*           HXX(KX) = HL(IX,KX)                                                             000354
00226     79*      86   SXX(KX) = SL(IX,KX)                                                             000356
00230     80*           TXX(NTUP+1) = TT                                                  CPHS 770      000361
00231     81*           CPXX(NTUP+1) = CPX                                                CPHS 780      000363
00232     82*           HXX(NTUP+1) = HX                                                  CPHS 790      000365
00233     83*           SXX(NTUP+1) = SX                                                  CPHS 800      000367
00234     84*           TT = TTS                                                          CPHS 820      000371
00235     85*           TLN = TLNS                                                        CPHS 830      000373
00236     86*           M = 1                                                                           000375
00237     87*           I = 1                                                                           000377
00240     88*           IF (TT .LT. TXX(M))  I = -1                                                     000400
00242     89*      87   IF (TT .GE. TXX(M) .AND. TT .LE. TXX(M+1))  GO TO 89                            000412
00244     90*           M = M + I                                                                       000430
00245     91*           IF (M .LT. NTUP + 1 .AND. M .GT. 0)  GO TO 87                                   000433
00247     92*           WRITE (JOUT,88) TT,M,NTUP,(I,TXX(I), I = 1,4)                                   000450
00261     93*      88   FORMAT (//50X,29H*CPHS* VARIABLE OUTSIDE TABLE//45X,4HTT =,1PE15.8              000470
00261     94*          1,5H  M =,I2,8H  NTUP =,I2//(50X,4HTXX(,I1,3H) =,E15.8))                         000470
00262     95*           GO TO 31                                                                        000470
00263     96*      89   S(J) = SXX(M) + (SXX(M+1)-SXX(M))*(TT-TXX(M))/(TXX(M+1)-TXX(M))                 000472
00264     97*           HO(J) = HXX(M) + (HXX(M+1)-HXX(M))*(TT-TXX(M))/(TXX(M+1)-TXX(M))                000506
00265     98*           CPUSED = CPXX(M)+(CPXX(M+1)-CPXX(M))*(TT-TXX(M))/(TXX(M+1)-TXX(M))              000514
00266     99*           CPSUM = CPSUM + CPUSED * EN(J,NPT)                                CPHS 940      000522
00267    100*           GO TO 32                                                          CPHS 950      000527
00270    101*      90   IF (IER .LT. 1)  WRITE (JOUT,904) TT                                            000531
00274    102*     904   FORMAT (//25X,60HERROR DURING LOW TEMPERATURE THERMO EVALUATION IN              000542
00274    103*          1 CPHS, TT =,F12.6,15H DEGREES KELVIN//)                                         000542
00275    104*           IER = 1                                                                         000542
00276    105*           GO TO 31                                                                        000544
00277    106*           END                                                                             000602
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  CPHS                                                                    DATE 101580       PAGE   [illegible]
     END OF COMPILATION:        NO  DIAGNOSTICS.

@HDG,P      DETON
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2FOR,S     DETON,DETON
HSA   E3 -10/15/80-13:06:18 (12,)

   SUBROUTINE DETON       ENTRY POINT 001331

   STORAGE USED: CODE(1) 001347; DATA(0) 000201; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSIS 000006
    0004    HOLCON 000010
    0005    POINTS 000335
    0006    MISC   001701
    0007    INDX   000041
    0010    PERF   000166
    0011    OUPT   000073
    0012    CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0013    NEWOF
    0014    HCALC
    0015    OUT1
    0016    EQLBRM
    0017    OUT2
    0020    OUT3
    0021    SAVE
    0022    NWDU$
    0023    NI02$
    0024    XPRR
    0025    EXP
    0026    SQRT
    0027    NI01$
    0030    NI03$
    0031    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    001305 1000L      0000    000035 11F        0001    000005 130G       0001    000040 146G       0001    000566 150L
    0001    000053 154G       0000    000044 190F       0000    000053 203F       0001    000255 205L       0001    000176 214G
    0000    000055 30F        0001    000651 341G       0001    000672 352G       0001    000711 362G       0001    000717 367G
    0001    000563 40L        0001    000750 401G       0001    000767 411G       0001    001004 422G       0001    001024 433G
    0001    001055 451G       0000    000114 46F        0001    001100 464G       0001    001115 475G       0000    000102 5F
    0001    001123 502G       0001    001142 514G       0001    001157 525G       0001    001176 535G       0001    001216 546G
    0000    000120 58F        0000    000123 68F        0001    000016 7L         0001    000615 860L       0000    000130 868F
    0001    001251 870L       0001    001270 902L       0000 R  000032 ALAM       0000 R  000017 ALFA       0006    000640 AM
    0006 R  000705 AM1        0006    001135 ANUM       0010    000133 APP        0003    000000 ATMN       0006    000004 ATOM
    0000 R  000022 A11        0000 R  000023 A12        0000 R  000024 A21        0000 R  000025 A22        0006    000514 B0
    0006    000545 B0P        0000 R  000026 B1         0000 R  000027 B2         0007    000036 CALCH      0007    000001 CONVG
    0006 R  000654 CP         0005 R  000032 CPR        0006 R  000706 CPR1       0006    000634 CPSUM      0012    000002 DEMAND
    0006    001560 DENS       0005 R  000064 DLVPT      0005 R  000047 DLVTP      0004    000000 END        0006    001700 ENLSAV
    0006    000000 ENN        0006    001676 ENNL       0006    001677 ENSAVE     0006    001414 ENTH       0010 L  000165 EOL
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DETON                                                                                                  DATE 101580        PAGE    2

 0006     000636 EQRAT        0011     000002 FA          0011     000003 FAP         0006     001445 FAZ         0011 R 000005 FB
 0011     000006 FC           0011 R 000007 FCP           0011     000012 FCST        0011     000014 FCV         0011     000015 FG
 0011     000017 FGE          0011     000020 FGV         0000 R 000000 FG1           0011 R 000021 FH           0011     000023 FI
 0011     000025 FIV          0011 R 000027 FM            0000 R 000001 FMM           0011 R 000031 FMT          0011     000050 FN
 0011 R 000052 FOUR           0006     001527 FOX         0011     000053 FP          0000 R 000003 FPP          0000 R 000002 FP1
 0000 R 000004 FRA            0000 R 000005 FRB           0011     000054 FS          0011 R 000056 FSV          0011 R 000067 FT
 0011     000061 FTK          0000 R 000006 FTT           0000 R 000007 FUD          0011     000063 FV          0011 R 000065 FVEL
 0011 R 000001 F13            0011     000000 F9X         0000 R 000014 GAM          0005 R 000101 GAMMAS       0004     000001 GAS
 0003     000001 GMET         0010 R 000150 GM1           0012     000000 GRAPH       0007 L 000003 HP           0006     000642 HPP
 0006 R 000637 HSUBO          0005 R 000000 HSUM          0010 R 000064 H1           0007     000030 IC          0007 I 000000 IDEBUG
 0004     000002 IE           0000 I 000011 II            0007     000015 IMAT        0000     000143 INJPS       0000 I 000010 IOF
 0007     000023 IONS         0007 I 000021 IP            0007     000037 IQSAVE      0007     000016 IQ1         0007 I 000034 IT
 0000 I 000012 ITR            0004 I 000003 IZERO         0000 I 000034 J            0007     000026 JLIQ        0012 I 000001 JOUT
 0007     000025 JSOL         0007     000031 JS1         0007 I 000005 K            0007     000014 KMAT        0004     000004 LANK
 0006     000463 LLMT         0007     000040 LSAVE       0004     000005 MOL         0007     000006 MOLES       0006 I 000707 NAME
 0007     000024 NC           0007     000023 NEWR        0007     000035 NFZ         0007     000012 NLM         0007 I 000017 NOF
 0007     000020 NOMIT        0007 I 000007 NP            0007 I 000011 NPT          0007 I 000027 NREAC        0007     000013 NS
 0007 I 000010 NT             0006 R 000635 OF            0011 R 000067 ONE          0004     000006 OX          0006 R 001644 OXF
 0005 R 000116 P              0003     000002 PATM        0010 R 000000 PCP          0006     001363 PECWT       0006 R 000633 PP
 0005 R 000217 PPP            0000 R 000013 PP1           0010 R 000101 PUB          0003 R 000003 RBAR         0003 R 000004 RBR
 0006     000644 RH           0006     001611 RHOP        0000 R 000020 RK           0006     001612 RMW         0010 R 000047 RRHO
 0000 R 000021 RR1            0006 R 001476 RTEMP         0003     000005 RVR         0007     000033 SHOCK       0005 R 000251 SONVEL
 0007     000004 SP           0005     000015 SSUM        0006     000001 SUMN        0006     000003 SO          0005 R 000150 T
 0000 R 000016 TEM            0006     000632 THIGH       0011 R 000070 THREE        0006     001643 TLN         0006     000630 TLOW
 0006     000627 TM           0006     000631 TMID        0005     000320 TOTN        0007 L 000002 TP           0006 R 000002 TT
 0005 R 000266 TTT            0000 R 000015 TT1           0010 R 000116 TUB          0011 R 000071 TWO          0000 R 000033 UD
 0005 R 000202 V              0005     000303 VLM         0006     000646 VMIN        0010 R 000032 VMOC         0007     000032 VOL
 0006     000650 VPLS         0005 R 000234 WM            0006     000652 WP          0000 R 000030 X1           0000 R 000031 X2
 0004     000007 ZERO         0011     000072 ZEROF


 00101      1*              SUBROUTINE DETON                                                                              000000
 00101      2*        C                                                                                       00343900    000000
 00101      3*        C     CHAPMAN-JOUGUET DETONATIONS                                                       00344000    000000
 00101      4*        C                                                                                                   000000
 00103      5*              COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                                       /CONSTS/    000000
 00104      6*              COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                                 /HOLCON/    000000
 00105      7*              COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                                   000000
 00105      8*             1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                              000000
 00105      9*             2 ,VLM(13),TOTN(13)                                                                            000000
 00106     10*              COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                                     000000
 00106     11*             1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                                 000000
 00106     12*             2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),                     /MISC/      000000
 00106     13*             3              CP(25)   ,AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),                             000000
 00106     14*             4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,                               000000
 00106     15*             5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                                          000000
 00107     16*              COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,K,MOLES,NP,NT,NPT,NLM,NS,                     /INDX/      000000
 00107     17*             1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,                  /INDX/      000000
 00107     18*             2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE                    /INDX/      000000
 00110     19*              COMMON /PERF/ PCP(26),VMOC(13),RRHO(13),H1(13),PUB(13),                           /PERF/      000000
 00110     20*             1              TUB(13),APP(13),GM1(13),EQL                                         /PERF/      000000
 00111     21*              COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),                   /OUPT/      000000
 00111     22*             1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR,                /OUPT/      000000
 00111     23*             2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,                  /OUPT/      000000
```

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J0111     24*          3            TWO,ZEROF                             /OUPT/     000000
00111     25*     C                                                                  000000
00112     26*             COMMON /CCC/ GRAPH,JOUT,DEMAND                             000000
00112     27*     C                                                                  000000
00113     28*           LOGICAL EQL,HP,TP                                            000000
00114     29*           DATA FG,/6HGAMMA1/,FMM/6HM/M1  /,FP1/6HP1 ATM/,FPP/6HP/P1  /, 000000
00114     30*          1 FRA/6HRHO/RH/,FRB,6HO1     /,FTT/6HT/T1  /,FUD/6HDET VE/    000000
00114     31*     C                                                                  000000
00125     32*           XX(A,X,B,Y,C,D) = (A*X-B*Y)/(A*C-B*D)                        000000
00125     33*     C                                                                  000000
00126     34*           IOF = 0                                                      000000
00127     35*           DO 9 II = 1,NREAC                                            000000
00132     36*         9 NAME(II,6)=IZERO                                             000005
G0134     37*           TT = 0.                                                      000007
00135     38*           IF (T(1) .LE. 0.0)  T(1) = RTEMP(1)                          000010
00137     39*         7 IOF = IOF+1                                                  000016
00140     40*           OF = OXF(IOF)                                                000021
00141     41*           CALL NEWOF                                                   000023
00142     42*           WRITE(JOUT,11)                                               000025
00144     43*        11 FORMAT(33H1DETONATION VELOCITY CALCULATIONS)                 000032
00145     44*           DO 902 IT = 1,NT                                             000032
00150     45*           TT = T(IT)                                                   000040
00151     46*           CALL HCALC                                                   000042
00152     47*           CALL OUT1                                                    000044
J0153     48*           DO 902 IP=1,NP                                               000046
00156     49*           H1(NPT) = RBAR*HSUBO                                         000055
00157     50*           TUB(NPT) = T(IT)                                             000061
00160     51*           PUB(NPT) = P(IP)                                             000063
00161     52*           CP(NPT) = RBAR*CPR1                                          000065
00162     53*           ITR= 0                                                       000070
00163     54*           TT= 3800.                                                    000071
00164     55*           PP1= 15.                                                     000073
00165     56*           PP = PP1*P(IP)                                               000075
00166     57*           HSUBO = H1(NPT)/RBAR + 0.750*T(IT)*PP1/AM1                   000077
00167     58*           TP = .FALSE.                                                 000105
00170     59*           HP= .TRUE.                                                   000106
00171     60*           CALL EQLBRM                                                  000110
00172     61*           HSUBO = H1(NPT)/RBAR                                         000117
00173     62*           HP= .FALSE.                                                  000122
00174     63*           IF (TT .LE. 0.0)  GO TO 902                                  000123
J0176     64*           GAM= GAMMAS(NPT)                                             000126
00177     65*           TT1 = TT/T(IT)                                               000137
00200     66*           II= 0                                                        000142
J0201     67*           TEM=TT1-.75*PP1/(CPR(NPT)*AM1)                               000143
0020.     68*           WRITE(JOUT,190)TT                                            000150
00205     69*       190 FORMAT(8HOT EST.=,F8.2/11X,4HP/P1,17X,4HT/T1)                000160
00206     70*           WRITE(JOUT,203) II,PP1,TT1                                   000160
00213     71*           DO 202 II = 1,3                                              000176
00216     72*           ALFA = WM(NPT)/AM1/TT1                                       000176
00217     73*           PP1= (1.+GAM)*(1.+(1.-4.*GAM*ALFA/(1.+GAM)**2)**.5)/(2.*GAM*ALFA) 000201
00220     74*           RK=PP1*ALFA                                                  000220
00221     75*           TT1= TEM+.5*PP1*GAM*(RK*RK-1.)/(AM1*CPR(NPT)*RK)             000222
00222     76*       202 WRITE(JOUT,203) II,PP1,TT1                                   000235
00230     77*       203 FORMAT (I5,2E20.8)                                           000247
00231     78*           TP= .TRUE.                                                   000247
00232     79*           TT = TT1*T(IT)                                               000251
```

ORIGINAL PAGE IS
OF POOR QUALITY

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00233     80*       205 ITR= ITR+1                                                        000255
00234     81*           PP = PP1*P(IP)                                                    000257
00235     82*           CALL EQLBRM                                                       000262
00236     83*           IF (NPT.EQ.0) GO TO 1000                                          000264
00240     84*           IF (TT .LE. 0.0)  GO TO 860                                       000266
00242     85*           GAM= GAMMAS(NPT)                                                  000272
00243     86*           RR1 = PP1*WM(NPT)/AM1/TT1                                         000274
00244     87*           A11= 1./PP1 + GAM*RR1*DLVPT(NPT)                                  000302
00245     88*           A12= GAM*RR1*DLVTP(NPT)                                           000310
00246     89*           A21= .5*GAM*(RR1**2-1.-DLVPT(NPT)*(1.+RR1**2))+DLVTP(NPT)-1.      000314
00247     90*           A22=-.5*GAM*DLVTP(NPT)*(RR1**2+1.)-WM(NPT)*CPR(NPT)               000330
00250     91*           B1= 1./PP1-1.+GAM*(RR1-1.)                                        000343
00251     92*           B2 = WM(NPT)*(HSUM(NPT) - H1(NPT)/RBAR)/TT - 0.5*GAM*(RR1**2 - 1.)  000353
00252     93*           X1 = XX(A22,B1,A12,B2,A11,A21)                                    000370
00253     94*           X2 = XX(A11,B2,A21,B1,A22,A12)                                    000400
00254     95*           ALAM= 1.                                                          000412
00255     96*           TEM = X1                                                          000414
00256     97*           IF(TEM.LT.0.)  TEM = -TEM                                         000416
00260     98*           IF(X2.GT.TEM)  TEM=X2                                             000423
00262     99*           IF (-X2.GT.TEM) TEM = -X2                                         000431
00264    100*           IF(TEM.GT.0.4) ALAM=.4/TEM                                        000437
00266    101*           PP1= PP1*EXP(X1*ALAM)                                             000446
00267    102*           TT1= TT1*EXP(X2*ALAM)                                             000456
00270    103*           TT = TT1*T(IT)                                                    000466
00271    104*           UD = RR1*SQRT(RBR*GAM*TT/WM(NPT))                                 000470
00272    105*           WRITE(JOUT,30)ITR,PP1,TT1,RR1,X1,X2                               000503
00302    106*        30 FORMAT 7HOITER =,I2,5X,6HP/P1 =,E15.8,5X,6HT/T1 =,E15.8,5X,10HRHO/   000516
00302    107*          1RHO1 =,E15.8/7X,13HDEL LN P/P1 =,E15.8,5X,13HDEL LN T/T1 =,E15.8)  000516
00302    108*     C     CONVERGENCE TEST                                                  000516
00303    109*           IF(ITR.LE.10 .AND. TEM.GT.0.5E-04)  GO TO 205                     000516
00305    110*           RRHO(NPT)=RR1                                                     000534
00306    111*           IF (CP(NPT) .LE. 0.0)  GO TO 40                                   000536
00310    112*           GM1(NPT) = CP(NPT)/(CP(NPT) - RBAR/AM1)                           000541
00311    113*           VMOC(NPT) = UD/SQRT(RBR*GM1(NPT)*T(IT)/AM1)                       000547
00312    114*           GO TO 150                                                         000561
00313    115*        40 GM1(NPT) = 0.                                                     000563
00314    116*           VMOC(NPT) = 0.                                                    000564
00315    117*       150 K = 0                                                             000566
00316    118*           IF (IP .EQ. NP .AND. IT .EQ. NT .OR. TT .LE. 0.0)  GO TO 860      000566
00320    119*           K = NPT                                                           000610
00321    120*           IF(NPT.NE.13)  GO TO 870                                          000612
00321    121*     C  OUTPUT                                                               000612
00323    122*       860 WRITE(JOUT,5)                                                     000615
00325    123*         5 FORMAT(1H1,42X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS )  000621
00326    124*           CALL OUT1                                                         000621
00327    125*           WRITE(JOUT,46)                                                    000623
00331    126*        46 FORMAT(13H UNBURNED GAS//)                                        000633
00332    127*           FMT(3) = F13                                                      000633
00333    128*           FMT(4) = FOUR                                                     000635
00334    129*           WRITE(JOUT,FMT) FP1,FB,FB,(PUB(J), J = 1,NPT)                     000637
00345    130*           FMT(4) = TWO                                                      000654
00346    131*           WRITE(JOUT,FMT) FT,FB,(TUB(J), J = 1,NPT)                         000656
00356    132*           WRITE(JOUT,FMT) FH,FB,(H1(J), J = 1,NPT)                          000675
00366    133*           DO 56 J = 1,NPT                                                   000717
00371    134*           V(J) = AM1                                                        000717
00372    135*       56  SONVEL(J) = SQRT(RBR*GM1(J)*TUB(J)/AM1)                           000720
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00374     136*          FMT(4) = THREE                                        000732
00375     137*          WRITE(JOUT,FMT) FM,FB,(V(J), J = 1,NPT)               000734
00405     138*          FMT(4) = FOUR                                         000753
00406     139*          WRITE(JOUT,FMT) FCP,(CP(J), J = 1,NPT)                000755
00415     140*          WRITE(JOUT,FMT) FG1,FB,FB,(GM1(J), J = 1,NPT)         000772
00426     141*          FMT(4) = ONE                                          001007
00427     142*          WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(J), J = 1,NPT)       001011
00437     143*          WRITE(JOUT,58)                                        001027
00441     144*       58 FORMAT(11H0BURNED GAS//)                              001034
00442     145*          FMT(3) = ONE                                          001034
00443     146*          CALL OUT2                                             001036
00444     147*          WRITE(JOUT,68)                                        001040
00446     148*       68 FORMAT(22H0DETONATION PARAMETERS //)                  001050
00447     149*          FMT(4) = THREE                                        001050
00450     150*          DO 70 J = 1,NPT                                       001055
00453     151*          V(J) = PPP(J)/PUB(J)                                  001055
00454     152*          PCP(J) = TIT(J)/TUB(J)                                001057
00455     153*       70 SONVEL(J) = SONVEL(J)*RRHO(J)                         001062
00457     154*          WRITE(JOUT,FMT) FPP,FB,FB,(V(J), J = 1,NPT)           001066
00470     155*          WRITE(JOUT,FMT) FTT,FB,FB,(PCP(J), J = 1,NPT)         001103
00501     156*          DO 73 J = 1,NPT                                       001123
00504     157*       73 V(J) = WM(J)/AM1                                      001123
00506     158*          FMT(4) = FOUR                                         001126
00507     159*          WRITE(JOUT,FMT) FMM,FB,FB,(V(J), J = 1,NPT)           001130
00520     160*          WRITE(JOUT,FMT) FRA,FRB,FB,(RRHO(J), J = 1,NPT)       001145
00531     161*          WRITE(JOUT,FMT) FM,FB,(VMOC(J), J = 1,NPT)            001162
00541     162*          FMT(4) = ONE                                          001201
00542     163*          WRITE(JOUT,FMT) FUD,FVEL,(SONVEL(J), J = 1,NPT)       001203
00552     164*          EQL=.TRUE.                                            001221
00553     165*          CALL OUT3                                             001223
00554     166*          IF (K .EQ. 0 .AND. IOF .EQ. NOF)  GO TO 1000          001225
00556     167*          IDEBUG = IDEBUG-13                                    001237
00557     168*          WRITE(JOUT,868)                                       001242
00561     169*      868 FORMAT(1H1)                                           001247
00562     170*          NPT = 0                                               001247
00563     171*      870 NPT = NPT + 1                                         001251
00564     172*          IF (K .EQ. 1)  K = -1                                 001253
00566     173*          CALL SAVE                                             001260
00567     174*          WRITE(JOUT,868)                                       001262
00571     175*      902 CONTINUE                                              001274
00574     176*          IF(IOF.GE.NOF)  GO TO 1000                            001274
00576     177*          IDEBUG = IDEBUG+13                                    001300
00577     178*          GO TO 7                                               001303
00600     179*     1000 TP = .FALSE.                                          001305
00601     180*          RETURN                                                001305
00602     181*          END                                                   001346

      END OF COMPILATION:          NO  DIAGNOSTICS.


@HDG,P      EQLBRM
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EQLBRM                                                                                    DATE 101580        PAGE     1

@FOR,S    EQLBRM,EQLBRM
HSA  E3 -10/15/80-13:06:23 (16,)

   SUBROUTINE EQLBRM     ENTRY POINT 003120

   STORAGE USED: CODE(1) 003136; DATA(0) 000461; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   CONSTS 000006
    0004   HOLCON 000010
    0005   POINTS 000335
    0006   SPECES 017106
    0007   MISC   001701
    0010   DOUBLE 001560
    0011   INDX   000041
    0012   PERF   000166
    0013   CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0014   CPHS
    0015   MATRIX
    0016   GAUSS
    0017   ALOG
    0020   NWDU$
    0021   NIO1$
    0022   NIO2$
    0023   EXP
    0024   NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   001202 100L     0001   001211 101L     0001   002172 1027G    0001   002222 1037G    0000   000223 110F
    0001   001452 111L     0001   001575 1115L    0001   001633 1116L    0001   001517 113L     0001   002503 1134G
    0001   001513 114L     0001   002511 1140G    0001   001542 115L     0001   002551 1154G    0001   001660 116L
    0001   002624 1160L    0001   002454 1165L    0001   002716 1171L    0000   000214 1183F    0001   002644 1205G
    0001   002676 1223G    0001   002741 1244G    0001   002046 13L      0001   001747 130L     0000   000321 136F
    0001   002660 143L     0000   000257 144F     0001   002263 147L     0001   002270 148L     0001   000116 151G
    0001   002516 153L     0001   002312 154L     0000   000265 156F     0001   002342 157L     0001   002401 158L
    0001   002437 159L     0001   002152 160L     0000   000277 161F     0001   000151 165G     0001   002630 165I
    0001   002650 166L     0000   000307 168F     0001   002616 169L     0001   002621 170L     0001   002725 171L
    0000   000111 172F     0001   000430 174L     0001   002062 183L     0001   003013 186L     0000   000165 1924F
    0001   003002 199L     0000   000326 201F     0001   001561 2115L    0001   000244 221G     0001   000277 232G
    0000   000072 244F     0001   000325 245G     0001   000332 251G     0001   000374 270G     0001   000406 277G
    0000   000220 306F     0001   000464 315G     0001   000512 324G     0001   000131 33L      0001   000613 360G
    0000   000103 373F     0001   002653 40L      0001   000721 416G     0001   000732 422G     0001   000155 43L
    0001   001003 445G     0001   001141 477G     0001   000125 499L     0001   001172 506G     0001   001252 531G
    0001   001413 600G     0001   000213 62L      0001   000251 63L      0001   001464 631G     0001   000302 67L
    0001   001625 673G     0001   001642 704G     0001   000342 72L      0001   001722 726G     0000   000107 73F
    0000   000140 74F      0001   001760 746G     0000   000324 771F     0000   000075 772F     0001   000412 773I
    0001   000524 774L     0001   000536 775L     0000   000144 776F     0001   000747 80L      0001   000766 83L
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0001     001023 84L      0001     001036 85L      0001     000571 871L     0001     003071 873L     0000     000117 874F
0001     001332 917L     0000     000146 923F     0000     000171 924F     0000     000210 925F     0001     000603 966L
0001     000622 968L     0001     000632 969L     0001     001111 97L      0001     000635 970L     0001     000644 973L
0000     000232 973F     0000     000250 974F     0001     000654 997L     0006 R   011052 A        0000 R   000061 AA
0012     000150 AEAT     0007     000640 AM       0000 R   000054 AMBDA    0000 R   000055 AMBDA1   0007     000705 AM1
0007     001135 ANUM     0012 R   000133 APP      0003     000000 ATMN     0007     000004 ATCM     0007 R   000614 BO
0007     000545 BOP      0011     000036 CALCH    0006     000000 COEF     0011 L   000001 CONVG    0005 R   000032 CPR
0007     000706 CPR1     0007 R   000634 CPSUM    0000 R   000040 CRITV    0007     000654 DATA     0000 R   000067 DELF
0006 R   010624 DELN     0013     000002 DEMAND   0007     001560 DENS     0000 R   000053 DLNT     0005 R   000064 DLVPT
0005 R   000047 DLVTP    0006 R   004312 EN       0004     000000 END      0000 R   000037 ENL      0006 R   010150 ENLN
0007     001700 ENLSAV   0007 R   000000 ENN      0007 R   001676 ENNL     0007     001677 ENSAVE   0000 R   000045 ENSOL
0007     001414 ENTH     0012     000165 EQL      0007 R   000636 EQRAT    0007     001445 FAZ      0000 R   000057 FNEG1
0000 R   000060 FNEG2    0007     001527 FOX      0010 D   000000 G        0005 R   000101 GAMMAS   0004     000001 GAS
0003     000001 GMET     0013     000000 GRAPH    0011 L   000003 HP       0007     000642 HPP      0007     000637 HSUBO
0005 R   000000 HSUM     0006 R   010376 HO       0000 I   000044 I        0011 L   000030 IC       0011 I   000000 IDEBUG
0004 I   000002 IE       0011 I   000015 IMAT     0000 I   000053 INC      0000     000421 INJPS    0011 L   000023 IONS
0011     000021 IP       0011     000037 IQSAVE   0011 I   000016 IQ1      0000 I   .00047 IQ2      0000 L   000034 ISING
0011     000005 ISV      0011     000034 IT       0000 I   000042 INUMB    0006 I   016266 IUSE     0004     000003 IZERO
0000 I   000043 J        0000 I   000070 JDELF    0000 I   000051 JJ       0000 I   000065 JKG      0011 I   000026 JLIQ
0013 I   000001 JOUT     0011 I   000025 JSOL     0011 I   000031 JS1      0000 I   000064 KG       0011 I   000014 KMAT
0011 I   000012 L        0004     000004 LANK     0007 I   000463 LLMT     0000 L   000035 LOGV     0011     000040 LSAVE
0004     000005 MOL      0011     000006 MOLES    0007     000707 NAME     0011 I   000024 NC       0000 I   000052 NEN
0011     000022 NEWR     0011     000035 NFZ      0011     000017 NOF      0011     000020 NOMIT    0011     000007 NP
0011 I   000011 NPT      0011     000027 NREAC    0011 I   000013 NS       0000 I   000000 NSPP1    0011     000010 NT
0000 I   000050 NTZERO   0000 I   000046 NUMB     0007     000635 OF       0004     000006 OX       0007     001644 OXF
0005     000116 P        0003     000002 PATM     0012     000000 PCP      0007     002363 PECWT    0007 R   000633 PP
0005 R   000217 PPP      0000 R   000001 PROW     0003     000003 RBAR     0003     000004 PBR      0007     000644 RH
0007     001611 RHOP     0000 L   000036 RITE     0007     001012 RMW      0007     001476 RTEMP    0003 R   000005 RVR
0006 R   004064 S        0011 L   000033 SHOCK    0000 R   000041 SIZEF    0006     016660 SLN      0005     000751 SONVEL
0011 L   000004 SP       0012     000047 SFIM     0000 R   000062 SS       0005 R   000015 SSUM     0006 R   015364 SUB
0012     000101 SUBAR    0000 D   000032 SUM      0007 R   000001 SUMN     0000 R   000056 SUM1     0012     000116 SUPAR
0007 R   000003 SO       0005 R   000150 T        0006 R   016514 TEMP     0007 R   000632 THIGH    0007 R   001643 TLN
0007 R   000630 TLOW     0007 R   000627 TM       0000 R   000066 TMELT    0007     000631 TMID     0000 R   000071 TN
0005 R   000320 TOTN     0011 L   000002 TP       0007 R   000002 TT       0005 R   000266 TTT      0005     000202 V
0012     000064 VACT     0005 R   000303 VLM      0007     000646 VMIN     0012     000032 VMOC     0011 L   000032 VOL
0007     000650 VPLS     0005 R   000234 WM       0007     000652 WP       0010 D   001510 X        0004     000007 ZERO
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00101      1*           SUBROUTINE EQLBRM                                              EQLN0002    000000
00101      2*     C                                                                                000000
00101      3*     C   ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES          EQLN0003    000000
00101      4*     C                                                                    EQLN0004    000000
00103      5*           COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                    /CONSTS/    000000
00104      6*           COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO              /HOLCON/    000000
00105      7*           COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                000000
00105      8*          1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)           000000
00105      9*          2 ,VLM(13),TOTN(13)                                                         000000
00105     10*     C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)            000000
00105     11*     C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)             000000
00106     12*           INCLUDE SPECPK                                                             000000
00112     13*           COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                  000000
00112     14*          1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,              000000
00112     15*          2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),   /MISC/     000000
00112     16*          3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),           000000
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      EQLBRM                                                                      DATE 101580        PAGE    3

 00112      17*           4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,                   000000
 00112      18*           5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                              000000
 00113      19*           COMMON /DOUBLE/ G(20,21), X(20)                              EQLN0013  000000
 00114      20*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,          /INDX/    000000
 00114      21*           1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/    000000
 00114      22*           2              NREAC,IC,JS1,VOL,SHOCK,T,NFZ,CALCH,IOSAVE,LSAVE     /INDX/    000000
 00115      23*           COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),          /PERF/    000000
 00115      24*           1              SUPAR(13),APP(13),AEAT(13),EQL                      /PERF/    000000
 00115      25*     C                                                                                    000000
 00116      26*              COMMON /CCC/ GRAPH,JOUT,DEMAND                                              000000
 00116      27*     C                                                                                    000000
 00117      28*           DIMENSION PROM(25)                                                             000000
 00120      29*           DOUBLE PRECISION G,SUM,X                                                       000000
 00121      30*           LOGICAL CONVG,HP,IC,IONS,ISING,LOGV,RITE,SHOCK,SP,TP,VOL                       000000
 00121      31*     C                                                                                    000000
 00122      32*           ENL = ENNL                                                                     000000
 00123      33*           RITE = .FALSE.                                                                 000001
 00124      34*           IF(IDEBUG.GT.0.AND.NPT.GE.IDEBUG)  RITE=.TRUE.                                 000002
 00126      35*           CRITV = 5.DE-6                                                                 000021
 00127      36*           SIZEF = 0.                                                                     000023
 00130      37*           ISING = .FALSE.                                                                000024
 00131      38*           LOGV = .FALSE.                                                                 000025
 00132      39*           IF (VOL)  PP = RVR*ENN*TT/VLM(NPT)                                             000026
 00134      40*           TLN = ALOG(TT)                                                                 000040
 00135      41*           CONVG = .FALSE.                                                                000044
 00136      42*           ITNUMB = 100                                                                   000045
 00137      43*           JS1 = 1                                                                        000047
 00140      44*           CALL CPHS                                                                      000051
 00141      45*           TM = ALOG(PP/ENN)                                                              000053
 00141      46*     C     IF(IC) PREVIOUS POINT HAD SINGULAR MATRIX                                      000053
 00142      47*           IF(IC)  GO TO 966                                                              000062
 00144      48*           IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33                                       000064
 00146      49*           L = L+1                                                                        000102
 00147      50*           IQ1 = IQ1+1                                                                    000105
 00150      51*           DO 499 J = 1,NS                                                                000116
 00153      52*           IF (A(L,J) .EQ.0.) GO TO 499                                                   000116
 00155      53*           EN(J,NPT) = 1.E-8                                                              000117
 00156      54*           ENLN(J) = -18.4206810                                                          000121
 00157      55*           IUSE(J) = 0                                                                    000123
 00160      56*       499 CONTINUE                                                                       000131
 00162      57*        33 IF(NPT.EQ.1.AND..NOT.SHOCK)  WRITE(JOUT,244)(LLMT(I),I=1,L)                    000131
 00171      58*       244 FORMAT (4HOPT ,14(5X,A4))                                                      000155
 00171      59*     C     BEGIN ITERATION                                                                000155
 00172      60*        43 IF(IC)  GO TO 1171                                                             000155
 00174      61*           IF (.NOT.CONVG)  GO TO 62                                                      000156
 00176      62*           SUMN = ENN                                                                     000166
 00177      63*           IF(JSOL.EQ.0)  GO TO 62                                                        000170
 00201      64*           ENSOL = EN(JSOL,NPT)                                                           000172
 00202      65*           EN(JSOL,NPT) = EN(JSOL,NPT)+EN(JLIQ,NPT)                                       000176
 00203      66*           IUSE(JLIQ) = -IUSE(JLIQ)                                                       000200
 00204      67*           IQ1 = IQ1-1                                                                    000202
 00205      68*           DLVTP(NPT) = 0.                                                                000205
 00206      69*           CPR(NPT) = 0.                                                                  000206
 00207      70*           GAMMAS(NPT) = 0.                                                               000207
 00210      71*           LOGV = .TRUE.                                                                  000210
 00211      72*        62 CALL MATRIX                                                    EQLN0048  000213
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00212     73*          NUMB = IQ1 - ITNUMB                                                            000214
00213     74*          IQ2 = IQ1 + 1                                                                  000217
00214     75*          IF(.NOT.CONVG)    GO TO 67                                                     000222
00216     76*          IF (LOGV.AND.JSOL.EQ.0) GO TO 63                                               000224
00220     77*          DO 182  I=1,L                                                     EQLN0140     000244
00223     78*      182 PROW(I) = G(IQ1,I)                                                             000244
00225     79*          IF (.NOT.LOGV) GO TO 67                                                        000246
00225     80*    C     LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT                               000246
00227     81*       63 G(IQ1,IQ2) = ENN                                                               000251
00230     82*          J = IQ1 - 1                                                                    000260
00231     83*          DO 777 I = 1,J                                                                 000270
00234     84*      777 G(I,IQ2) = G(I,IQ1)                                                            000277
00236     85*       67 IF(.NOT.RITE)  GO TO 72                                                        000302
00240     86*          WRITE(JOUT,772) NUMB                                                           000303
00243     87*      772 FORMAT (11H0ITERATION  ,I3,6X,7HMATRIX //)                                     000325
00244     88*          DO 911 I=1,IMAT                                                   EQLN0051     000325
00247     89*      911 WRITE(JOUT,73) (G(I,J), J = 1,KMAT)                                            000325
00256     90*       72 IF(CONVG)  IMAT=IMAT-1                                                         000342
00260     91*          J = IMAT                                                                       000346
00261     92*          CALL GAUSS                                                                     000350
00262     93*          IF (J .NE. IMAT)  GO TO 774                                                    000352
00264     94*          IF(.NOT.RITE)  GO TO 773                                                       000355
00266     95*          WRITE(JOUT,373)(LLMT(I),I=1,L)                                                 000363
00274     96*      373 FORMAT (7H0PI     ,9(A4,10X))                                                  000377
00275     97*          WRITE(JOUT,73)(X(I),I=1,IMAT)                                                  000377
00303     98*       73 FORMAT (9E14.6)                                                   EQLN0062     000412
00304     99*      773 IF(.NOT.CONVG)  GO TO 85                                                       000412
00306    100*          IF(.NOT.LOGV)  GO TO 174                                                       000413
00310    101*          IF(JLIQ.NE.0) EN(JSOL,NPT)=ENSOL                                               000421
00312    102*          GO TO 171                                                                      000426
00313    103*      174 SUM = 0.                                                          EQLN0148     000430
00314    104*          DO 175 J=1,L                                                      EQLN0149     000431
00317    105*      175 SUM = SUM + PROW(J)*X(J)                                                       000464
00321    106*          DLVTP(NPT) = 1.+G(IQ2,IQ1)/ENN-SUM/ENN  - X(IQ))                  EQLN0151     000470
00322    107*          CPR(NPT) = G(IQ2,IQ2)                                             EQLN0152     000502
00323    108*          DO 176 J=1,IQ1                                                    EQLN0153     000512
00326    109*      176 CPR(NPT) = CPR(NPT) - G(IQ2,J)*X(J)                                            000512
00330    110*          LOGV = .TRUE.                                                     EQLN0155     000520
00331    111*          GO TO 62                                                                       000522
00331    112*    C  SINGULAR MATRIX                                                                   000522
00332    113*      774 IF(.NOT.CONVG)  GO TO 775                                                      000524
00332    114*    C     IF(ISING)   SINGULAR ONCE                                                      000524
00332    115*    C     IF(IC)      SINGULAR TWICE                                                     000524
00334    116*          WRITE(JOUT,172)                                                                000525
00336    117*      172 FORMAT(28H0DERIVATIVE MATRIX SINGULAR )                                        000532
00337    118*          IC = .TRUE.                                                                    000532
00340    119*          GO TO 1171                                                                     000534
00341    120*      775 IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 871                   000536
00343    121*          WRITE(JOUT,874)                                                                000562
00345    122*      874 FORMAT(96H0LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE               000567
00345    123*         1BEEN INCLUDED ON AN INSERT CARD, RESTART )                                     000567
00346    124*          GO TO 873                                                                      000567
00347    125*      871 WRITE(JOUT,74)                                                                 000571
00351    126*       74 FORMAT(16H0SINGULAR MATRIX)                                                    000575
00352    127*          IF(IC)  GO TO 873                                                              000575
00354    128*          IF (ISING) GO TO 357                                                           000577
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00356    129*           NTZERO = 0                                                                000601
00357    130*       966 DO 970 JJ = 1, NS                                                         000603
00362    131*           IF(IUSE(JJ)) 970,968,967                                                  000613
00365    132*       967 IF (EN(JJ,NPT))  969,873,969                                              000616
00370    133*       968 IF (EN(JJ,NPT) .GT. 0.0)  GO TO 969                                       000622
00372    134*           EN(JJ,NPT) = 1.0E-6                                                       000624
00373    135*           ENLN(JJ) = -13.815511                                                     000626
00374    136*           GO TO 970                                                                 000630
00375    137*       969 NTZERO = NTZERO+1                                                         000632
00376    138*       970 CONTINUE                                                                  000637
00400    139*           IF(.NOT.IC)  GO TO 971                                                    000637
00402    140*           IC = .FALSE.                                                              000641
00403    141*           GO TO 43                                                                  000642
00404    142*       971 ISING = .TRUE.                                                            000644
00405    143*           WRITE(JOUT,776)                                                           000645
00407    144*       776 FORMAT (8H0RESTART)                                                       000652
00410    145*           GO TO 43                                                                  000652
00411    146*       997 IF(NIZERO.NE.L-1.OR.EQRAT.GT.1.00001.OR.EQRAT.LT..99999) GO TO 873        000654
00413    147*           ENN=0.                                                                    000710
00414    148*           NEN = 0                                                                   000711
00415    149*           DO 83  I=1,L                                                              000721
00420    150*           JJ = 0                                                                    000724
00421    151*           DO 80  J=1,NS                                                             000732
00424    152*           IF (EN(J,NPT) .EQ. 0.0 .OR. A(I,J) .EQ. 0.0)  GO TO 80                    000732
00426    153*           IF (JJ .NE. 0)  GO TO 83                                                  000742
00430    154*           JJ = J                                                                    000744
00431    155*        80 CONTINUE                                                                  000752
00433    156*           NEN = NEN+1                                                               000752
00434    157*           EN(JJ,NPT) = BO(I)/A(I,JJ)                                                000755
00435    158*        83 CONTINUE                                                                  000767
00437    159*           IF(NEN.LT.NTZERO)  GO TO 873                                              000767
00441    160*           CONVG = .TRUE.                                                            000773
00442    161*           IC = .TRUE.                                                               000775
00443    162*           HSUM(NPT) = 0.                                                            000776
00444    163*           DO 84  J=1,NS                                                             001003
00447    164*           IF (EN(J,NPT) .LE. 0.0)  GO TO 84                                         001003
00451    165*           ENN = EN(J,NPT)+ENN                                                       001005
00452    166*           ENLN(J) = ALOG(EN(J,NPT))                                                 001010
00453    167*           HSUM(NPT) = HSUM(NPT) + EN(J,NPT)*HO(J)                                   001016
00454    168*        84 CONTINUE                                                                  001025
00456    169*           TM = ALOG(PP/ENN)                                                         001025
00457    170*           GO TO 43                                                                  001034
00460    171*        85 ITNUMB= ITNUMB-1                                              EQLN0068    001036
00461    172*           IF (ITNUMB .LT. 30)  CRITV = CRITV + 2.50E-7                              001040
00461    173*     C     OBTAIN CORRECTIONS TO THE ESTIMATES                            EQLN0070    001040
00463    174*           JJ = L + 1                                                                001047
00464    175*           IF(VOL)  X(IO2)=X(IO1)                                                    001060
00466    176*           IF(TP)  X(IO2)=0.                                                         001066
00470    177*           DLNT= X(IO2)                                                  EQLN0072    001073
00471    178*           SUM = X(IO1)                                                              001076
00472    179*           IF(.NOT.VOL) GO TO 97                                                     001101
00474    180*           X(IO1) = 0.                                                               001103
00475    181*           SUM =    -DLNT                                                            001105
00476    182*        97 DO 101 J=1,NS                                                             001111
00501    183*           IF (IUSE(J)) 101,98,100                                                   001145
00504    184*        98 DELN(J) = HO(J)*DLNT-HO(J)+S(J)-ENLN(J)-TM+SUM                            001151
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00505    185*            DO 99 I = 1,L                                                          001172
00510    186*         99 DELN(J) = DELN(J) + A(I,J)*X(I)                                        001172
00512    187*            GO TO 101                                                              001200
00513    188*        100 DELN(J) = X(JJ)                                                        001202
00514    189*            JJ = JJ + 1                                                            001205
00515    190*        101 CONTINUE                                                   EQLN0079    001213
00517    191*            AMBDA= 1.                                                  EQLN0080    001213
00520    192*            AMBDA1= 1.                                                 EQLN0081    001215
00521    193*            SUM = X(IQ1)                                                           001216
00522    194*            IF(SUM.LT.0.)  SUM=-SUM                                                001222
00524    195*            IF(DLNT.GT.SUM)  SUM=DLNT                                              001230
00526    196*            IF(-DLNT.GT.SUM)  SUM=-DLNT                                            001236
00530    197*            DO 917 J=1,NS                                              EQLN0084    001252
00533    198*            IF (IUSE(J).NE.0) GO TO 917                                            001252
00535    199*            IF (EN(J,NPT) .GT. 0.0 .AND. DELN(J) .GT. SUM)  SUM = DELN(J)          001253
00537    200*            IF (EN(J,NPT) .GT. 0.0 .OR. DELN(J) .LE. 0.0)  GO TO 917               001272
00541    201*            SUM1 = (-9.212-ENLN(J)+ ENL)/(DELN(J)-X(IQ1))                          001306
00542    202*            IF(SUM1.LT.0.)  SUM1=-SUM1                                             001316
00544    203*            IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1                                      001323
00546    204*        917 CONTINUE                                                   EQLN0089    001334
00550    205*            IF(SUM.GT.2.)AMBDA=2./SUM                                  EQLN0090    001334
00552    206*            IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1                                    001344
00554    207*            IF(.NOT.RITE)  GO TO 111                                               001352
00556    208*            WRITE(JOUT,923) IT,ENN, ENL,PP,TM,AMBDA                                001354
00566    209*        923 FORMAT (3HOT=,E15.8,6H  ENN=,E15.8,7H  ENNL=E15.8,5H  PP=,E15.8,       001367
00566    210*          1 9H  LN P/N=E15.8,8H  AMBDA=E15.8 )                                     001367
00567    211*            IF(VOL)  WRITE(JOUT,1924) VLM(NPT)                                     001367
00573    212*       1924 FORMAT(8H VOLUME=,E15.8,2HCC)                                          001401
00574    213*            WRITE(JOUT,924)                                                        001401
00576    214*        924 FORMAT(1H0,18X,2HNI,12X,5HLN NI,8X,9HDEL LN NI,10X,4HH/RT,9X,4HSO/     001413
00576    215*          1R,12X,6H-G0/RT,9X,5H-G/RT  )                                            001413
00577    216*            DO 926 J=1,NS                                                          001413
00602    217*            FNEG1 = S(J)-H0(J)                                                     001413
00603    218*            FNEG2 = FNEG1                                                          001415
00604    219*            IF(IUSE(J).EQ.0)  FNEG2=FNEG2-ENLN(J)-TM                               001416
00606    220*        926 WRITE(JOUT,925) SUB(J,1),SUB(J,2),SUB(J,3),EN(J,NPT),ENLN(J),          001424
00606    221*          A                DELN(J),H0(J),S(J),FNEG1,FNEG2                          001424
00623    222*        925 FORMAT (1X,3A4,7E15.6)                                                 001444
00624    223*            WRITE(JOUT,110)                                                        001444
00626    224*        110 FORMAT(1H0)                                                            001452
00626    225*     C      APPLY CORRECTIONS TO ESTIMATES                             EQLN0096    001452
00627    226*        111 SUM = 0.                                                               001452
00630    227*            DO 113 J=1,NS                                              EQLN0099    001453
00633    228*            IF (IUSE(J)) 113,112,114                                               001464
00636    229*        112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)                              EQLN0100    001467
00637    230*            EN(J,NPT) = 0.                                             EQLN0101    001473
00640    231*            IF (ENLN(J) + 18.4206810 .LE. ENL)  GO TO 113                          001474
00642    232*            EN(J,NPT) = EXP(ENLN(J))                                               001500
00643    233*            SUM = SUM+EN(J,NPT)                                                    001506
00644    234*            GO TO 113                                                              001511
00645    235*        114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)                                001513
00646    236*        113 CONTINUE                                                               001521
00650    237*            SUMN = SUM                                                             001521
00651    238*            IF (TP) GO TO 115                                          EQLN0104    001523
00653    239*            TLN= TLN+AMBDA*DLNT                                        EQLN0105    001525
00654    240*            TT     = EXP(TLN)                                          EQLN0106    001531
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00655     241*           JS1 = 1                                                               001535
00656     242*           CALL CPHS                                                             001537
00657     243*       115 IF(VOL) GO TO 2115                                                    001542
00661     244*           ENL = ENL+AMBDA*X(IQ1)                                                001543
00662     245*           ENN = EXP(ENL)                                                        001553
00663     246*           GO TO 1115                                                            001557
00664     247*      2115 ENN = SUMN                                                            001561
00665     248*           ENNL = ALOG(ENN)                                                      001562
00666     249*           PP = RVR*TT*ENN/VLM(NPT)                                              001566
00667     250*      1115 TM = ALOG(PP/ENN)                                                     001575
00670     251*           IF (LLMT(L).NE.IE) GO TO 116                                          001603
00670     252*     C     CHECK ON REMOVING IONS                                                001603
00672     253*           DO 1116 J = 1,NS                                                      001625
00675     254*           IF (A(L,J).EQ.0.) GO TO 1116                                          001625
00677     255*           IF (EN(J,NPT).GT.0.) GO TO 116                                        001627
00701     256*      1116 CONTINUE                                                              001642
00703     257*           DO 1118  J=1,NS                                                       001642
00706     258*      1118 IF (A(L,J) .NE. 0.0)  IUSE(J) = - 10000                               001642
00711     259*           L = L-1                                                               001650
00712     260*           IQ1 = IQ1-1                                                           001653
00713     261*           GO TO 43                                                              001656
00713     262*     C     TEST FOR CONVERGENCE                                       EQLN0110   001656
00714     263*       116 IF (ITNUMB.EQ.0) GO TO 13                                  EQLN0112   001660
00716     264*           IF (AMBDA.LT.1.) GO TO 43                                  EQLN0113   001661
00720     265*           SUM = (ENN-SUMN)/ENN                                                  001674
00721     266*           IF (SUM.LT.0.) SUM = -SUM                                             001704
00723     267*           IF (SUM .GT. CRITV)  GO TO 43                                         001712
00725     268*           DO 130 J=1,NS                                              EQLN0115   001722
00730     269*           IF (IUSE(J).LT.0) GO TO 130                                           001722
00732     270*           AA= DELN(J)/SUMN                                                      001725
00733     271*           IF(AA.LT.0.)  AA=-AA                                                  001730
00735     272*           IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)                                   001735
00737     273*           IF (AA .GT. CRITV)  GO TO 43                                          001742
00741     274*       130 CONTINUE                                                              001751
00741     275*     C     CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS                   001751
00743     276*           TOTN(NPT) = 0.                                                        001751
00744     277*           SSUM(NPT) = 0.                                                        001753
00745     278*           DO 183 J=1,NS                                              EQLN0133   001760
00750     279*           IF(IUSE(J).LT.0)  GO TO 183                                           001760
00752     280*           TOTN(NPT) = TOTN(NPT) + EN(J,NPT)                                     001762
00753     281*           SS = S(J)                                                             001765
00754     282*           IF(IUSE(J).EQ.0)  SS=SS-ENLN(J)-TM                                    001767
00756     283*           SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)                                    001775
00757     284*       183 CONTINUE                                                   EQLN0136   002004
00761     285*           IF(.NOT.SP.OR.NPT.EQ.1)  GO TO 13                                     002004
00763     286*           SS = SSUM(NPT) -S0                                                    002014
00764     287*           IF(SS.LT.(-0.00005).OR.SS.GT.0.00005)  GO TO 43                       002020
00766     288*           IF(RITE)  WRITE(JOUT,1183)  SS                                        002035
00772     289*      1183 FORMAT(12H0DELTA S/R =,E15.8)                                         002046
00773     290*        13 CONVG= .TRUE.                                              EQLN0117   002046
00774     291*           IF(TT    .LT.TLOW.OR.TT    .GT.THIGH)WRITE(JOUT,306)TT,NPT             002047
01001     292*       306 FORMAT(17H0THE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,I5)EQLN0119   002074
01002     293*           IF(ITNUMB.NE.0) GO TO 160                                             002074
01004     294*           WRITE(JOUT,973) NPT                                                   002076
01007     295*       973 FORMAT (//5X,69H100 ITERATIONS DID NOT SATISFY THE CONVERGENCE REQ    002104
01007     296*          1UIREMENTS FOR POINT,I3/)                                              002104
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01010    297*          WRITE (JOUT,974) TT                                                    002104
01013    298*      974 FORMAT (5X,'aaaa TEMPERATURE=',F12.4,' aaaa')                          002112
01014    299*          IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 873           002112
01016    300*          WRITE(JOUT,874)                                                        002137
01020    301*          TT = T(1)                                                              002144
01021    302*          RETURN                                                                 002146
01021    303*    C     CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.               002146
01022    304*      160 IF(NC.EQ.0) GO TO 143                                                  002152
01024    305*          SIZEF = 0.                                                             002153
01025    306*          INC = 0                                                                002154
01026    307*          DO 170 J = 1,NS                                                        002172
01031    308*          IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-10000) GO TO 170                     002172
01033    309*          INC = INC + 1                                                          002204
01034    310*          IF(RITE)  WRITE(JOUT,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),     002207
01034    311*         1IUSE(J),EN(J,NPT)                                                      002207
01047    312*      144 FORMAT (1H0,3A4,2F10.3,3X,5HIUSE=,I4,E15.7)                            002241
01050    313*          IF (EN(J,NPT))  146,148,169                                            002241
01053    314*      146 IF (J.NE.JSOL .AND. J .NE.JLIQ) GO TO 147                              002244
01055    315*          JSOL = 0                                                               002260
01056    316*          JLIQ = 0                                                               002261
01057    317*      147 IQ1 = IQ1 - 1                                                          002263
01060    318*          EN(J,NPT) = 0.                                                         002265
01061    319*          GO TO 166                                                              002266
01062    320*      148 KG = 1                                                                 002270
01063    321*          IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154                                    002271
01065    322*          IF (J .EQ. 1 .OR. IUSE(J) .NE. -IUSE(J-1))  GO TO 153                  002274
01067    323*          KG = -1                                                                002307
01070    324*      154 JKG = J + KG                                                           002312
01071    325*          IF (EN(JKG,NPT).LT.0.) GO TO 170                                       002314
01073    326*          TMELT = TEMP(INC,1)                                                    002321
01074    327*          IF (TMELT .EQ. TEMP(INC+KG,2))  GO TO 158                              002324
01076    328*          TMELT = TEMP(INC,2)                                                    002330
01077    329*          IF (TMELT .EQ. TEMP(INC+KG,1))  GO TO 157                              002332
01101    330*          WRITE(JOUT,156)                                                        002334
01103    331*      156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER  )        002342
01103    332*    C  JTH SPECIES A SOLID (EN=0), (J+KG)TH SPECIES A LIQUID (EN IS +)           002342
01104    333*     157  IF (TT .GT. TMELT .OR. (TP .AND. TT .EQ. TMELT))  GO TO 169            002342
01106    334*          IF (TP .OR. TT .LE. TMELT - 150.0)  GO TO 1165                         002361
01110    335*          JSOL = J                                                               002373
01111    336*          JLIQ = JKG                                                             002375
01112    337*          GO TO 159                                                              002377
01112    338*    C  JTH SPECIES A LIQUID(EN=0), (J+KG)TH SPECIES A SOLID (EN IS +)            002377
01113    339*     158  IF (TT .LT. TMELT .OR. (TP .AND. TT .EQ. TMELT))  GO TO 169            002401
01115    340*          IF (TP .OR. TT .GE. TMELT + 150.0)  GO TO 1165                         002420
01117    341*          JSOL = JKG                                                             002432
01120    342*          JLIQ = J                                                               002434
01121    343*      159 TLN = ALOG (TMELT)                                                     002437
01122    344*          TT = TMELT                                                             002442
01123    345*          EN(JKG,NPT) = .5 * EN(JKG,NPT)                                         002444
01124    346*          EN(J,NPT) = EN(JKG,NPT)                                                002451
01125    347*          GO TO 165                                                              002452
01125    348*    C  WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN                            002452
01126    349*     1165 EN(J,NPT) = EN (JKG, NPT)                                              002454
01127    350*          IUSE(J) = -IUSE(J)                                                     002457
01130    351*          IUSE (JKG) = -IUSE(JKG)                                                002461
01131    352*          EN(JKG,NPT)= 0.                                                        002464
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01132    353*         WRITE(JOUT,161) (SUB(JKG,I), I = 1,3),(SUB(J,I), I = 1,3)                              002471
01144    354*    161  FORMAT (10X,22HPHASE CHANGE, REPLACE ,3A4,6H WITH ,3A4)                                002514
01145    355*         GO TO 40                                                                               002514
01146    356*     153 IF (TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GO TO 169                              002516
01150    357*         IF (TT.GT.TEMP(INC,2)) GO TO 169                                                       002533
01152    358*         SUM = 0.                                                                               002542
01153    359*         DO 167 I = 1,L                                                                         002551
01156    360*    167  SUM = SUM + A(I,J)*X(I)                                                                002551
01160    361*         DELF = HO(J)-S(J)-SUM                                                                  002555
01161    362*         IF(RITE)  WRITE(JOUT,168)DELF,SIZEF                                                    002563
01166    363*     168 FORMAT (17H GO-SUM(AIJ*PI) =E15.7,10X,18HPREVIOUS DELTA G =,E15.7)                     002574
01167    364*         IF(DELF.GE.SIZEF .OR. DELF.GE.0.) GO TO 169                                            002574
01171    365*         SIZEF = DELF                                                                           002611
01172    366*         JDELF = J                                                                              002613
01173    367*     169 IF(INC.EQ.NC) GO TO 1160                                                               002616
01175    368*     170 CONTINUE                                                                               002624
01177    369*    1160 IF (SIZEF.EQ.0.) GO TO 143                                                             002624
01201    370*         J = JDELF                                                                              002625
01202    371*     165 IO1 = IO1 + 1                                                                          002630
01203    372*         WRITE(JOUT,136) (SUB(J,I), I = 1,3)                                                    002632
01211    373*    136  FORMAT (10X,4HADD ,3A4)                                                                002650
01212    374*     166 IUSE(J) = - IUSE(J)                                                                    002650
01213    375*      40 CONVG = .FALSE.                                                                        002653
01214    376*         JS1 = 1                                                                                002653
01215    377*         CALL CPHS                                                                              002655
01216    378*     143 TN = NUMB                                                                              002660
01217    379*         IF (.NOT. SHOCK)  WRITE(JOUT,771) NPT,(X(I), I = 1,L),TN                               002662
01230    380*     771 FORMAT (I3,14F9.3)                                                                     002703
01231    381*         JS1 = 1                                                                                002703
01232    382*         IF(TP.AND.CONVG)  CALL CPHS                                                            002705
01234    383*         ITNUMB = 100                                                                           002712
01235    384*         GO TO 43                                                             EQLN0126          002714
01235    385*    C    CALCULATE EQUILIBRIUM PROPERTIES                                     EQLN0128          002714
01236    386*    1171 DLVPT(NPT) = -1.                                                                       002716
01237    387*         DLVTP(NPT) = 1.                                                                        002720
01240    388*         CPR(NPT) = CPSUM                                                                       002721
01241    389*         GO TO 199                                                                              002723
01242    390*     171 SUM = 0.                                                                               002725
01243    391*         DO 179 J = 1,L                                                       EQLN0167          002726
01246    392*    179  SUM = SUM + PROW(J)*X(J)                                                               002741
01250    393*         DLVPT(NPT) = -2.*SUM/ENN+ X(IO1)                                     EQLN0170          002745
01251    394*         IF (JLIQ .EQ. 0)  GO TO 199                                                            002754
01253    395*         IUSE(JLIQ) = -IUSE(JLIQ)                                                               002756
01254    396*         HSUM(NPT) = HSUM(NPT)+EN(JLIQ,NPT)*(HO(JLIQ)-HO(JSOL))                                 002761
01255    397*         IO1 = IO1+1                                                                            002772
01256    398*         GAMMAS(NPT) = -1./DLVPT(NPT)                                                           002775
01257    399*         GO TO 186                                                                              003000
01260    400*     199 GAMMAS(NPT) = -1./(DLVPT(NPT)+(DLVTP(NPT)**2)*ENN/CPR(NPT))          EQLN0171          003002
01261    401*     186 TTT(NPT) = TT                                                        EQLN0178          003013
01262    402*         ENNL = ENL                                                                             003015
01263    403*         PPP(NPT) = PP                                                                          003017
01264    404*         VLM(NPT) = RVR*ENN*TT/PP                                                               003021
01265    405*         HSUM(NPT) = HSUM(NPT)*TT                                                               003026
01266    406*         WM(NPT) = 1./ENN                                                     EQLN0180          003031
01267    407*         IF (.NOT. RITE)  RETURN                                                                003035
01271    408*         WRITE(JOUT,201) NPT,APP(NPT),PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),                        003042
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OF POOR QUALITY

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 01271    409.          1 CPR(NPT),OLVPT(NPT),OLVTP(NPT),GAMMAS(NPT),VLM(NPT)                  003092
 01307    410.      201 FORMAT (7HOPOINT=I3,3X,4HPCP=E13.6,3X,2HP=E13.6,3X,2HT=E13.6,3X,4H     003065
 01307    411.         1H/R=E13.6,3X,4HS/R=E13.6//3X,3HMW=E13.6,3X,5HCP/R=E13.6,3X,6HDLVPT   003065
 01307    412.         2=E13.6,3X,6HOLVTP=E13.6,3X,9HGAMMA(S)=E13.6,3X,2HV=,E13.6)          003065
 01310    413.          RETURN                                                              003065
 01310    414.    C     ERROR. SET TT=0                                                     003065
 01311    415.      873 TT=0.                                                               003071
 01312    416.          NPT = NPT-1                                                         003071
 01313    417.          RETURN                                                              003074
 01314    418.          END                                                                 003135

       END OF COMPILATION:          NO  DIAGNOSTICS.

 @HDG,P      FROZEN
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@FOR,S   FROZEN,FROZEN
HSA  E3 -10/15/80-13:06:33 (10.)

   SUBROUTINE FROZEN    ENTRY POINT 000345

   STORAGE USED: CODE(1) 000360; DATA(0) 000041; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSIS 000006
    0004    POINTS 000335
    0005    SPECES 017106
    0006    MISC   001701
    0007    INDX   000041

   EXTERNAL REFERENCES (BLOCK, NAME)

    0010    CPHS
    0011    ALOG
    0012    EXP
    0013    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001     000066 1356     0001     000251 2076     0001     000022 51L      0001     000050 55L      0001     000120 60L
    0001     000165 11L      0001     000313 901L     0001     000321 903L     0005     011052 A        0006     000640 AM
    0006     000705 AM1      0006     001135 ANUM     0003     000000 ATMN     0006     000004 ATOM     0006     000514 BO
    0006     000545 BOP      0007     000036 CALCH    0000 R   000005 CC       0005     000000 COEF     0007 L   000001 CONVG
    0004 R   000032 CPR      0006     000706 CPR1     0006 R   000634 CPSUM    0006     000654 DATA     0005     010624 DELN
    0006     001560 DENS     0000 R   000007 DLNT     0004 R   000064 DLVPT    0004 R   000047 DLVTP    0005 R   004312 EN
    0005     010150 ENLN     0006     001700 ENLSAV   0006     000000 ENN      0006     001676 ENNL     0006     001677 ENSAVE
    0006     001414 ENTH     0006     000636 FORAT    0006     001445 FAZ      0006     001527 FOX      0004 R   000101 GAMMAS
    0003     000001 GMET     0007 L   000003 HP       0006     000642 HPP      0006 R   000637 HSUBO    0004 R   000000 HSUM
    0005 R   010376 HO       0007     000030 IC       0007     000000 IDEBUG   0007     000015 IMAT     0000 I   000010 INC
    0000     000015 INJPS    0007     000023 IONS     0007     000021 IP       0007     000037 IOSAVE   0007     000016 IOI
    0007     000005 ISV      0007     000034 IT       0005 I   016266 IUSE     0000 I   000004 J        0007     000026 JLIO
    0007     000025 JSOL     0007 I   000031 JS1      0007     000014 KMAT     0006     000463 LLMT     0007     000040 LSAVE
    0007     000006 MOLES    0006     000707 NAME     0007 I   000024 NC       0007     000022 NEWR     0007 I   000035 NFZ
    0007     000012 NLM      0007     000017 NOF      0007     000020 NOMIT    0007     000007 NP       0007 I   000011 NPT
    0007     000027 NREAC    0007 I   000013 NS       0000 I   000000 NSPP1    0007     000010 NT       0006     000635 OF
    0006     001644 OXF      0004     000116 P        0003     000002 PATM     0006     001363 PECWT    0006 R   000633 PP
    0004 R   000217 PPP      0003     000003 RBAR     0003     000004 RBR      0006     000644 RH       0006     001611 RHOP
    0006     001612 RMW      0000 R   000001 RNV      0006     001476 RTEMP    0003 R   000005 RVR      0005 R   004064 S
    0007     000033 SHOCK    0005     016660 SLN      0004     000251 SONVEL   0007 L   000004 SP       0000 R   000006 SS
    0004 R   000015 SSUM     0005     015364 SUB      0000 R   000003 SUMH     0006     000001 SUMN     0000 R   000002 SUMS
    0006 R   000003 SO       0004     000150 T        0005 R   016514 TEMP     0006     000632 THIGH    0006 R   001643 TLN
    0006 R   000630 TLOW     0006     000627 TM       0006     000631 TMID     0004 R   000320 TOTN     0007     000002 TP
    0006 R   000002 TT       0004 R   000266 TTT      0004     000202 V        0004 R   000303 VLM      0006     000646 VMIN
    0007 L   000032 VOL      0006     000650 VPLS     0004 R   000234 WM       0006     000652 WP
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00101        1*            SUBROUTINE FROZEN                                              FRO20002   000000
00101        2*       C                                                                   FRO20001   000000
00101        3*       C    (FROZEN COMPOSITION EXPANSION ONLY)                            FRO20004   000000
00101        4*       C                                                                   FRO20005   000000
00103        5*            COMMON /CONSTS/ AIMN,GMET,PATM,RBAR,RBR,RVR                    /CONSTS/   000000
00104        6*            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)               000000
00104        7*            1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)         000000
00104        8*            2 ,VLM(13),TOTN(13)                                                       000000
00104        9*       C    COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)           000000
00104       10*       C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)           000000
00105       11*            INCLUDE SPECPR                                                            000000
00111       12*            COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                 000000
00111       13*            1             BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,             000000
00111       14*            2             HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),  /MISC/     000000
00111       15*            3             DATA(25),AMI,CPRI,NAME(25,6),ANUM(23,6),PECWT(25),          000000
00111       16*            4             ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,           000000
00111       17*            5             RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                      000000
00112       18*            COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,  /INDX/  000000
00112       19*            1             KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ, /INDX/   000000
00112       20*            2             NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE   /INDX/   000000
00112       21*       C                                                                              000000
00113       22*            LOGICAL CONVG,HP,SP,VOL                                                   000000
00113       23*       C                                                                              000000
00114       24*            CONVG = .FALSE.                                                           000000
00115       25*            TLN = ALOG(TT)                                                            000000
00116       26*            IF (VOL)  RNV = RVR/(VLM(NPT)*WM(NFZ))                                    000004
00120       27*        51  SUMS=0.                                                                   000022
00121       28*            SUMH = 0.                                                                 000022
00122       29*            JS1 = 1                                                                   000023
00123       30*            J = NPT                                                                   000025
00124       31*            NPT = NFZ                                                                 000027
00125       32*            CALL CPHS                                                                 000031
00126       33*            CC = CPSUM                                                                000033
00127       34*            IF(.NOT.VOL)  GO TO 55                                                    000035
00131       35*            CC = CPSUM-1./WM(NFZ)                                                     000037
00132       36*            PP = RNV*TT                                                               000044
00133       37*        55  NPT = J                                                                   000050
00134       38*            DO 60 J = 1,NS                                                            000051
00137       39*            IF (EN(J,NFZ) .LE. 0.0)  GO TO 60                                         000066
00141       40*            SS = S(J)                                                                 000070
00142       41*            IF(IUSE(J).EQ.0)  SS=SS-ALOG(EN(J,NFZ)*PP*WM(NFZ))                        000072
00144       42*            SUMS = SUMS+SS*EN(J,NFZ)                                                  000105
00145       43*            IF (CONVG.OR.HP)  SUMH=SUMH+HO(J)*EN(J,NFZ)                               000111
00147       44*        60  CONTINUE                                                      FRO20058    000122
00151       45*            IF (CONVG) GO TO 81                                           FRO20059    000122
00153       46*            IF(SP)  DLNT=(SUMS-SO)/CC                                                 000124
00155       47*            IF(HP)  DLNT=(SUMH-HSUBO/TT)/CC                                           000132
00157       48*            TLN=TLN-DLNT                                                  FRO20061    000141
00160       49*            IF(DLNT.LT.0.) DLNT=-DLNT                                                 000144
00162       50*            IF(DLNT.LT.0.5E-4)  CONVG=.TRUE.                                          000151
00164       51*            TT = EXP(TLN)                                                             000157
00165       52*            GO TO 51                                                      FRO20063    000163
00166       53*        81  TTT(NPT)= TT                                                              000165
00167       54*            SSUM(NPT)= SUMS                                                           000167
00170       55*            HSUM(NPT)= TT*SUMH                                                        000171
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00171     56*        GAMMAS(NPT)= CPSUM/(CPSUM-1./WM(NFZ))                   000173
00172     57*        VLM(NPT) = RVR*TT/(WM(NFZ)*PP)                          000202
00173     58*        WM(NPT) = WM(NFZ)                                       000210
00174     59*        DLVPT(NPT) = -1.                                        000212
00175     60*        DLVTP(NPT) = 1.                                         000214
00176     61*        TOTN(NPT) = TOTP(NFZ)                                   000215
00177     62*        PPP(NPT) = PP                                           000217
00200     63*        CPR(NPT)= CPSUM                                         000221
00201     64*        IF (TT.LT.(TLOW-150.))GO TO 903                         000223
00203     65*        IF (NC .EQ. 0)  RETURN                                  000230
00205     66*        INC =0                                                  000244
00206     67*        DO 901 J = 1,NS                                         000251
00211     68*        IF (IUSE(J) .EQ. 0 .OR. IUSE(J) .EQ. - 10000)  GO TO 901 000251
00213     69*        INC = INC+1                                             000263
00214     70*        IF (EN(J,NFZ) .LE. 0.0)  GO TO 901                      000267
00216     71*        IF (TT.LT.TEMP(INC,1)-50. .OR. TT.GT.TEMP(INC,2)+50.)  GO TO 903  000272
00220     72*    901 CONTINUE                                                000315
00222     73*        RETURN                                                  000315
00223     74*    903 TT=0.                                                   000321
00224     75*        NPT= NPT-1                                              000321
00225     76*        RETURN                                                  000324
00226     77*        END                                           FRO20084  000357

      END OF COMPILATION:        NO  DIAGNOSTICS.

 @HDG,P      GAMEFF
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@FOR,S    GAMEFF,GAMEFF
MSA  E3 -10/15/80-13:06:42 (2,)

   SUBROUTINE GAMEFF     ENTRY POINT 000176

   STORAGE USED: CODE(1) 000217; DATA(0) 000044; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003   XPRR
    0004   SQRT
    0005   NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    000036 10L        0001    000025 1056        0001    000132 20L        0001    000152 50L        0000 R 000002 ANK
    0000 R 000006 CFA         0000 R 000005 CGAM         0000 R 000001 G           0000 R 000004 GM          0000 R 000003 GP
    0000 I 000000 I           0000    000014 INJP$

00101        1*             SUBROUTINE GAMEFF (V,GAMMAS,A,N,M)                         000025
00103        2*             DIMENSION A(13),GAMMAS(13),M(13),V(13)                     000025
00103        3*       C                                                                000025
00104        4*             DO 50 I = 2,N                                              000025
00107        5*             G = GAMMAS(I)                                              000025
00110        6*             ANK = +1.0                                                 000026
00111        7*             IF (G .GT. 1.0)  GO TO 10                                  000030
00113        8*             G = 1.0010                                                 000033
00114        9*         10  GP = G + 1.0                                               000036
00115       10*             GM = G - 1.0                                               000040
00116       11*             CGAM = SQRT(G)*(2.0/GP)**(GP/(2.0*GM))                     000043
00117       12*             CFA = CGAM*SQRT(2.0*G*(1.0 - (1.0/A(I))**(GM/G))/GM)       000063
00120       13*             IF (ABS(V(I) - CFA) .LE. 5.0E-5)  GO TO 50                 000110
00122       14*             IF (G .LT. 2.0)  GO TO 20                                  000115
00124       15*             IF (ANK .LT. 0.0)  GO TO 50                                000121
00126       16*             ANK = -1.0                                                 000124
00127       17*             G = GAMMAS(I)                                              000126
00130       18*             GO TO 10                                                   000130
00131       19*         20  G = G + ANK*(V(I) - CFA)                                   000132
00132       20*             IF (G .GT. 1.0)  GO TO 10                                  000136
00134       21*             IF (ANK .LT. 0.0)  GO TO 50                                000141
00136       22*             ANK = -1.0                                                 000144
00137       23*             G = GAMMAS(I)                                              000146
00140       24*             GO TO 10                                                   000150
00141       25*         50  M(I) = G                                                   000152
00143       26*             RETURN                                                     000157
00144       27*              END                                                       000216

   END OF COMPILATION:         NO  DIAGNOSTICS.
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BHOG,P GAUSS

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@FOR,S    GAUSS,GAUSS
HSA  E3 -10/15/80-13:06:54 (7,)

   SUBROUTINE GAUSS      ENTRY POINT 000411

   STORAGE USED: CODE(1) 000431; DATA(0) 000126; BLANK COMMON(2) 000000

    COMMON BLOCKS:

     0003    DOUBLE 001560
     0004    INDX   000041

   EXTERNAL REFERENCES (BLOCK, NAME)

     0005    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001     000107 10L        0001     000011 1106       0001     000043 1206       0001     000062 1276       0001     000130 1526
     0001     000161 1676       0001     000204 1776       0001     000115 18L        0001     000256 2106       0001     000257 2136
     0001     000141 22L        0001     000361 23L        0001     000333 2316       0001     000167 31L        0001     000275 45L
     0001     000303 47L        0001     000340 51L        0001     000020 8L         0001     000101 9L         0004     000036 CALCH
     0000 D   000000 COEFX      0004     000001 CONVG      0003 D   000000 G          0004     000003 HP         0000 I   000056 I
     0004     000030 IC         0004     000000 IDEBUG     0000     000071 INJPS      0004     000023 IONS       0004     000021 IP
     0004     000037 IQSAVE     0004     000016 IQ1        0004     000005 ISV        0004     000034 IT         0004 I   000015 IUSE
     0000 I   000054 IUSE1      0000 I   000057 J          0004     000026 JLIQ       0004     000025 JSOL       0004     000031 JS1
     0000 I   000061 K          0004     000014 KMAT       0004     000040 LSAVE      0004     000006 MOLES      0004     000024 NC
     0004     000022 NEWR       0004     000035 NFZ        0004     000012 NLM        0000 I   000055 NN         0004     000017 NOF
     0004     000020 NOMIT      0004     000007 NP         0004     000011 NPT        0004     000027 NREAC      0004     000013 NS
     0004     000010 NT         0004     000033 SHOCK      0004     000004 SP         0000 D   000050 SUM        0000 R   000060 TEMP
     0004     000002 TP         0004     000032 VOL        0003 D   001510 X          0000 D   000052 Z


 00101      1*           SUBROUTINE GAUSS                                                                  000000
 00103      2*           COMMON/DOUBLE/G(20,21),X(20)                                                      000000
 00104      3*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,     /INDX/        000000
 00104      4*          1              KMAT,IUSE,IQ1,NCF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,   /INDX/        000000
 00104      5*          2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE     /INDX/        000000
 00105      6*           DOUBLE PRECISION COEFX(20),G,SUM,X,Z                                              000000
 00105      7*     C     BEGIN ELIMINATION OF NNTH VARIABLE                                  00205000      000000
 00106      8*           IUSE1=IUSE+1                                                        00203600      000000
 00107      9*           DO 45 NN = 1,IUSE                                                                 000002
 00112     10*           IF (NN .NE. IUSE)  GO TO 8                                                        000011
 00114     11*           IF (G(NN,NN))  31,23,31                                                           000014
 00114     12*     C     SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW                          00205600      000014
 00117     13*         8 DO 18 I=NN,IUSE                                                                   000020
 00122     14*           COEFX(I) = 1.0E38                                                                 000047
 00123     15*           IF(G(I,NN).EQ.0.)  GO TO 18                                                       000051
 00125     16*           COEFX(I) = 0.                                                                     000054
 00126     17*           DO 10 J=NN,IUSE1                                                                  000062
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OF POOR QUALITY

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00131    18*            SUM = G(I,J)                                                         000062
00132    19*            IF(SUM.LT.0.)  SUM=-SUM                                              000064
00134    20*            IF(J.NE.NN)  GO TO 9                                                 000072
00136    21*            Z = SUM                                                              000075
00137    22*            GO TO 10                                                             000077
00140    23*          9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM                                    000101
00142    24*         10 CONTINUE                                                             000111
00144    25*            COEFX(I) = COEFX(I)/Z                                                000111
00145    26*         18 CONTINUE                                                             000121
00147    27*            TEMP = 1.0E38                                                        000121
00150    28*            I=0                                                       00207200   000123
00151    29*            DO 22 J = NN,IUSE                                                    000130
00154    30*            IF (COEFX(J) .GE. TEMP)  GO TO 22                                    000130
00156    31*            TEMP = COEFX(J)                                                      000134
00157    32*            I=J                                                       00207600   000136
00160    33*         22 CONTINUE                                                  00207700   000143
00162    34*            IF (I .EQ. 0)  GO TO 23                                              000143
00162    35*     C      INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH  00208200   000143
00162    36*     C      VARIABLE FROM THE REMAINING EQUATIONS                     00208300   000143
00162    37*     C       INTERCHANGE EQUATIONS I AND NN                           00208500   000143
00164    38*            IF (NN .EQ. I)  GO TO 31                                             000145
00166    39*            DO 30 J = NN,IUSE1                                                   000150
00171    40*            Z=G(I,J)                                                  00208900   000161
00172    41*            G(I,J)=G(NN,J)                                            00209000   000162
00173    42*         30 G(NN,J) = Z                                                          000164
00173    43*     C      DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH  00209300   000164
00173    44*     C      VARIABLE FROM THE REMAINING EQUATIONS                     00209400   000164
00175    45*         31 K = NN + 1                                                00209600   000167
00176    46*            DO 36 J = K, IUSE1                                        00209700   000171
00201    47*            IF(G(NN,NN).EQ.0.)  GO TO 23                                         000204
00203    48*         36 G(NN,J) = G(NN,J)/G(NN,NN)                                           000207
00205    49*            IF (K .EQ. IUSE1)  GO TO 45                                          000214
00207    50*            DO 44 I = K,IUSE                                                     000217
00212    51*            DO 44 J = K,IUSE1                                                    000257
00215    52*         44 G(I,J) = G(I,J) - G(I,NN)*G(NN,J)                                    000257
00220    53*         45 CONTINUE                                                  00210500   000300
00220    54*     C      BACKSOLVE FOR THE VARIABLES                               00210700   000300
00222    55*            K = IUSE                                                  00211000   000300
00223    56*         47 J = K + 1                                                 00211100   000303
00224    57*            X(K) = 0.000                                              00203800   000305
00225    58*            SUM = 0.0                                                 00211200   000312
00226    59*            IF (IUSE .LT. J)  GO TO 51                                           000313
00230    60*            DO 50 I = J,IUSE                                                     000316
00233    61*         50 SUM = SUM + G(K,I)*X(I)                                              000333
00235    62*         51 X(K) = G(K,IUSE1) - SUM                                              000340
00236    63*            K = K - 1                                                 00211800   000350
00237    64*            IF (K .NE. 0)  GO TO 47                                              000353
00241    65*            RETURN                                                               000355
00242    66*         23 IUSE = IUSE-1                                                        000361
00243    67*            RETURN                                                               000363
00244    68*            END                                                                  000430

     END OF COMPILATION:        NO  DIAGNOSTICS.
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       GAUSS                                                        DATE 101580     PAGE    3
    aHDG,P     HCALC
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HCALC                                                                                  DATE 101580        PAGE      1

@FOR,S    HCALC,HCALC
HSA  E3 -10/15/80-13:06:58 (11,)

   SUBROUTINE HCALC      ENTRY POINT 000526

   STORAGE USED: CODE(1) 000542; DATA(0) 000066; BLANK COMMON(2) 000000

    COMMON BLOCKS:

   0003     CONSIS 000006
   0004     HOLCON 000010
   0005     POINTS 000101
   0006     SPECES 017106
   0007     MISC   001701
   0010     INDX   000041
   0011     CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

   0012     CPHS
   0013     ALOG
   0014     NWDU$
   0015     NI02$
   0016     NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

   0001     000070 1436       0001     000107 15L        0001     000131 16L        0001     000145 185G       0001     000154 1726
   0001     000162 1776       0001     000204 2106       0001     000275 2276       0001     000170 30L        0001     000026 4L
   0001     000177 50L        0001     000432 500L       0001     000251 55L        0001     000265 56L        0001     000307 70L
   0001     000467 75L        0000     000010 76F        0001     000477 80L        0000     000024 85F        0001     000037 9L
   0001     000312 90L        0006 R 011052 A           0004 I 000001 AG          0007 R 000640 AM          0007 R 000705 AM1
   0000 R 000002 ANN         0007 R 001135 ANUM        0003     000000 ATMN       0007     000004 ATOM       0004 I 000004 BLK
   0007     000514 BO         0007     000545 BOP        0010 L 000036 CALCH      0006     000000 COEF       0010     000001 CONVG
   0005     000032 CPR        0007 R 000706 CPR1        0007 R 000634 CPSUM      0007 R 000654 DATA        0006     010624 DELN
   0011     000002 DEMAND     0007     001560 DENS       0005     000064 DLVPT      0005     000047 DLVTP      0006 R 004312 EN
   0004     000000 END        0000 R 000007 ENJ         0006     010150 ENLN       0007     001700 ENLSAV     0007     000000 ENN
   0007     001676 ENNL       0007     001677 ENSAVE     0007 R 001414 ENTH       0007     000636 EORAT      0007 I 001445 FAZ
   0007 I 001527 FOX         0003     000001 GMET       0011     000000 GRAPH      0010     000003 HP         0007 R 000642 HPP
   0007 R 000637 HSUBO       0005     000000 HSUM       0006 R 010376 HO         0000 I 000005 I           0010     000030 IC
   0010     000000 IDEBUG     0004     000002 IE         0010     000015 IMAT       0000     000044 INJPS      0010     000023 IONS
   0010     000021 IP         0010     000037 IQSAVE     0010     000016 IO1        0000 I 000006 IS          0010     000005 ISV
   0010     000034 IT         0006 I 016266 IUSE        0004 I 000003 IZERO      0010 I 000031 J           0010     000026 JLIO
   0011 I 000001 JOUT        0010     000025 JSOL       0000 I 000004 K          0010     000014 KMAT       0010 I 000012 L
   0007 I 000463 LLMT        0010     000040 LSAVE      0004     000005 MOL        0010 L 000006 MOLES      0000 I 000003 N
   0007 I 000707 NAME        0010     000024 NC         0010     000022 NEWR       0010     000035 NFZ        0010     000017 NOF
   0010     000020 NOMIT      0010     000007 NP         0010 I 000011 NPT        0010 I 000027 NREAC      0010 I 000013 NS
   0000 I 000000 NSPP1       0010     000010 NT         0007 I 001135 NUM        0007 R 000635 OF          0004 I 000006 OX
   0007     001644 OXF        0003     000002 PATM       0007 R 001363 PECWT      0007 R 000633 PP          0003 R 000003 RBAR
   0003     000004 RBR        0007     000644 RH         0007     001611 RHOP       0007 R 001612 RMW         0007 R 001476 RTEMP
   0003     000005 RVR        0006 R 004064 S           0010 L 000033 SHOCK      0006     016660 SLN        0010     000004 SP
   0005 R 000015 SSUM        0006     015364 SUB        0007     000001 SUMN       0007     000003 SD         0006 R 016514 TEMP
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0007 R 000632 THIGH       0007 R 001643 TLN         0007 R 000630 TLOW       0007 R 000627 TM         0007   000631 TMID
0010   000002 TP          0000 R 000001 TSAVE       0007 R 000002 TT         0007   000646 VMIN       0010 L 000032 VOL
0007   000650 VPLS        0007 R 000652 WP          0004   000007 ZERO


00101      1*           SUBROUTINE HCALC                                                                000000
00101      2*     C  CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS                               000000
00103      3*           COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                       /CONSTS/      000000
00104      4*           COMMON /HOLCON/ END,AG,IE,IZERO,BLK,MOL,OX,ZERO                   /HOLCON/      000000
00105      5*           COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                     000000
00105      6*     C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                 000000
00105      7*     C   1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150),                  000000
00106      8*           INCLUDE SPECPK                                                                  000000
00112      9*           COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                       000000
00112     10*          1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                   000000
00112     11*          2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),      /MISC/       000000
00112     12*          3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),                000000
00112     13*          4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,                 000000
00112     14*          5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                            000000
00113     15*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,      /INDX/       000000
00113     16*          1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,   /INDX/       000000
00113     17*          2              NREAC,IC,J,VOL,SHOCK,IT,NF2,CALCH,IOSAVE,LSAVE       /INDX/       000000
00113     18*     C                                                                                     000000
00114     19*              COMMON /CCC/ GRAPH,JOUT,DEMAND                                               000000
00114     20*     C                                                                                     000000
00115     21*           DIMENSION NUM(25,6)                                                             000000
00116     22*           EQUIVALENCE (ANUM,NUM)                                                          000000
00117     23*           INTEGER AG,BLK,FAZ,FOX,OX                                                       000000
00120     24*           LOGICAL CALCH,MOLES,SHOCK,VOL                                                   000000
00121     25*           TSAVE = TT                                                                      000000
00122     26*           IF (AM(1) .GT. 0.0 .AND. AM(2) .GT. 0.0)  GO TO 4                               000001
00124     27*           AM1= AM(2)                                                                      000015
00125     28*           IF (AM(2) .LE. 0.0)  AM1 = AM(1)                                                000017
00127     29*           GO TO 9                                                                         000024
00130     30*         4 AM1=(OF+1.)*AM(1)*AM(2)/(AM(1)+OF*AM(2))                                        000026
00131     31*         9 TM = 0.                                                                         000037
00132     32*           IF(PP.GT.0.) TM = ALOG(PP*AM1)                                                  000037
00134     33*           SSUM(NPT) = 0.                                                                  000051
00135     34*           HPP(1) = 0.                                                                     000053
00136     35*           HPP(2) = 0.                                                                     000054
00137     36*           HSUBO = 0.                                                                      000055
00140     37*           CPR1 = 0.                                                                       000056
00141     38*           ANN = (1.+OF)                                                                   000057
00141     39*     C     LOOP ON REACTANTS. IF OXIDANT, K = 1, IF FUEL, K = 2.                           000057
00142     40*           DO 900 N=1,NREAC                                                                000070
00145     41*           K=2                                                                             000070
00146     42*           IF(FOX(N).EQ.OX)K=1                                                             000072
00150     43*           IF (NAME(N,6).NE.IZERO) GO TO 90                                                000077
00152     44*           IF(.NOT.CALCH)   GO TO 15                                                       000102
00154     45*           TT = RTEMP(N)                                                                   000104
00154     46*     C  IS TT IN RANGE                                                                     000104
00155     47*        15 IF (SHOCK)  GO TO 16                                                            000107
00157     48*           IF (TT .LT. TLOW - 100.0 .OR. TT .GT. THIGH + 1000.0)  GO TO 75                 000110
00161     49*        16 J=NUM(N,6)                                                                      000131
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     HCALC                                                                    DATE 101580          PAGE      3

  00162      50*           IF (J.NE.0)  GO TO 90                                            000136
  00164      51*           DO 10 J=1,L                                                      000145
  00167      52*        10 DATA(J) = 0.0                                                    000145
  00171      53*           DO 30 I=1,S                                                      000154
  00174      54*           IF (ANUM(N,I) .LE. 0.0)  GO TO 50                                000154
  00176      55*           DO 20 J=1,L                                                      000162
  00201      56*        20 IF (LLMT(J) .EQ. NAME(N,I))  GO TO 30                            000162
  00204      57*        30 DATA(J) = DATA(J) + ANUM(N,I)                                    000170
  00206      58*        50 IS=0                                                             000177
  00207      59*           DO 70 J=1,NS                                                     000177
  00212      60*           IF(IUSE(J).EQ.0)GO TO 55                                         000204
  00214      61*           IS = IS+1                                                        000206
  00215      62*           IF(FAZ(N).EQ.AG)GO TO 70                                         000212
  00217      63*           IF(TT.GT.TEMP(IS,2).AND.TEMP(IS,2).NE.THIGH)  GO TO 70           000215
  00221      64*           IF(TT.LT.TEMP(IS,1).AND.TEMP(IS,1).NE.TLOW)  GO TO 70            000232
  00223      65*           GO TO 56                                                         000247
  00224      66*        55 IF(FAZ(N).NE.AG.AND.FAZ(N).NE.BLK)  GO TO 70                     000251
  00226      67*        56 DO 60 I=1,L                                                      000265
  00231      68*        60 IF (A(I,J) .NE. DATA(I))  GO TO 70                               000275
  00234      69*           NUM(N,6)=J                                                       000303
  00235      70*           GO TO 90                                                         000305
  00236      71*        70 CONTINUE                                                         000310
  00240      72*           GO TO 80                                                         000310
  00241      73*        90 IF (MOLES)        ENJ = PECWT(N)/WP(K)                           000312
  00243      74*           IF (.NOT.MOLES)        ENJ = PECWT(N)/RMW(N)                     000325
  00245      75*           ENJ = ENJ/ANN                                                    000332
  00246      76*           IF(K.EQ.1)  ENJ = ENJ*OF                                         000335
  00250      77*           IF (NAME(N,6).NE.IZERO) GO TO 500                                000343
  00252      78*           I = NS                                                           000346
  00253      79*           NS = J                                                           000350
  00254      80*           TLN = ALOG(TT)                                                   000352
  00255      81*           IF(.NOT.CALCH)  EN(J,NPT) = ENJ                                  000356
  00257      82*           CALL CPHS                                                        000363
  00260      83*           NS = I                                                           000366
  00261      84*           IF (HO(J).GT.-.01 .AND. HO(J).LT..01) HO(J) = 0.                 000371
  00263      85*           RTEMP(N) = TT                                                    000411
  00264      86*           IF(VOL) HO(J)=HO(J)-1.                                           000413
  00266      87*           ENTH(N) = RBAR*TT*HO(J)                                          000421
  00267      88*           CPR1 = CPR1 + CPSUM                                              000426
  00270      89*       500 HSUBO = HSUBO + ENTH(N)*ENJ                                      000432
  00271      90*           HPP(K) = HPP(K)+ENTH(N)*ENJ                                      000440
  00272      91*       900 SSUM(NPT) = SSUM(NPT) + ENJ*(S(J) - ALOG(ENJ) - TM)              000444
  00274      92*           TT = TSAVE                                                       000456
  00275      93*           HSUBO = HSUBO/RBAR                                               000460
  00276      94*           RETURN                                                           000463
  00277      95*        75 WRITE(JOUT,76)                                                   000467
  00301      96*        76 FORMAT (//20X,57HREACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA  000473
  00301      97*          1IN HCALC/)                                                       000473
  00302      98*           RETURN                                                           000473
  00303      99*        80 WRITE(JOUT,85) N                                                 000477
  00306     100*        85 FORMAT (//20X,I2,42HTH REACTANT IS NOT IN THERMO DATA IN HCALC/) 000504
  00307     101*           RETURN                                                           000504
  00310     102*           END                                                              000541

     END OF COMPILATION:         NO  DIAGNOSTICS.
     HCALC
@HDG,P      LISTIT                                              DATE 101580        PAGE     4

@PRT,S    LISTIT
FURPUR 28R1H E33 S74T11 10/15/80 13:07:03
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LISTIT                                                                DATE 101580        PAGE    1

SEVIGNBIN208*TPFS(D).LISTIT
       1        @FOR,S LEWIS.BLOCK1,LEWIS.BLOCK1
       2        @FOR,S LEWIS.CPHS,LEWIS.CPHS
       3        @FOR,S LEWIS.DETON,LEWIS.DETON
       4        @FOR,S LEWIS.EQLBRM,LEWIS.EQLBRM
       5        @FOR,S LEWIS.FROZEN,LEWIS.FROZEN
       6        @FOR,S LEWIS.GAMEFF,LEWIS.GAMEFF
       7        @FOR,S LEWIS.GAUSS,LEWIS.GAUSS
       8        @FOR,S LEWIS.HCALC,LEWIS.HCALC
       9        @FOR,S LEWIS.LTCPHS,LEWIS.LTCPHS
      10        @FOR,S LEWIS.MAIN,LEWIS.MAIN
      11        @FOR,S LEWIS.MATRIX,LEWIS.MATRIX
      12        @FOR,S LEWIS.OUT1,LEWIS.OUT1
      13        @FOR,S LEWIS.REACT,LEWIS.REACT
      14        @FOR,S LEWIS.RKTOUT,LEWIS.RKTOUT
      15        @FOR,S LEWIS.ROCKET,LEWIS.ROCKET
      16        @FOR,S LEWIS.RREAD,LEWIS.RREAD
      17        @FOR,S LEWIS.SAVE,LEWIS.SAVE
      18        @FOR,S LEWIS.SEARCH,LEWIS.SEARCH
      19        @FOR,S LEWIS.SHCK,LEWIS.SHCK
      20        @FOR,S LEWIS.THERMP,LEWIS.THERMP
      21        @FOR,S LEWIS.VARFMT,LEWIS.VARFMT
      22        @BRKPT PRINTS

@HDG,P          LTCPHS
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@FOR,S     LTCPHS,LTCPHS
HSA  E3 -10/15/80-13:07:03 (2,)

   SUBROUTINE LTCPHS    ENTRY POINT 000205

   STORAGE USED: CODE(1) 000221; DATA(0) 000130; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   CONSTS 000006
    0004   LOWTH  001201

   EXTERNAL REFERENCES (BLOCK, NAME)

    0005   PAGIT
    0006   CHRSIZ
    0007   GOUT
    0010   RDATAI
    0011   RDCHAR
    0012   NDCODS
    0013   RDATAF
    0014   NIO1S
    0015   NIO2S
    0016   NERR3S

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   000006 10L       0000   000072 100F      0001   000025 1246      0001   000045 1326      0001   000111 1446
    0001   000113 147G      0001   000124 1566      0001   000026 20L       0001   000051 30L       0001   000122 46L
    0003   000000 ATMN      0004 R 000361 CPL       0003   000001 GMET      0004 R 000551 HL        0000 I 000066 I
    0004 I 001131 ILSP      0000 I 000024 IMN       0000   000107 INJPS     0000 I 000000 INLTMN    0000 I 000012 ISNMN
    0000 I 000015 ITMPMN    0000 I 000067 J         0000 I 000071 K         0004 I 000000 NLTSP     0000 I 000070 NT
    0003   000002 PATM      0003 R 000003 RBAR      0003   000004 RBR       0000 R 000062 RDUM      0003   000005 RVR
    0004 R 000741 SL        0004 R 000001 SUBLT     0004 R 000171 TL


 00101      1*          SUBROUTINE LTCPHS                                             LTCP  10     000000
 00101      2*     C                                                                               000000
 00101      3*     C       PROCESS LOW TEMPERATURE  CP,H,S  (VIA MIPS I/O)                         000000
 00101      4*     C                                                                               000000
 00101      5*     C       DIMENSION MIPS OUTPUT ARRAYS                                            000000
 00103      6*             DIMENSION INLTMN(10),ISNMN(3),ITMPMN(7),IMN(5,6),RDUM(4)                000000
 00103      7*     C                                                                               000000
 00104      8*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                   /CONSTS/     000000
 00105      9*          COMMON /LOWTH/ NLTSP,SUBLT(40,3),TL(40,3),CPL(40,3),HL(40,3),   /LOWTH/      000000
 00105     10*         1               SL(40,3),ILSP(40)                              /LOWTH/      000000
 00105     11*     C                                                                               000000
 00105     12*     C       SET DATA FOR MIPS OUTPUT                                                000000
 00106     13*             DATA INLTMN/24HTYPE THE NUMBER OF LOW T,                                000000
 00106     14*         1    36HEMPERATURE SPECIES TO BE ENTERED    /                               000000
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00110     15*              DATA ISNMN/18HTYPE SPECIES NAME /                        000000
00112     16*              DATA ITMPMN/42HTYPE NUMBER OF TEMPERATURES,THIS SPECIES<4/ 000000
00114     17*              DATA IMN/36HTYPE  TL,CPL,HL,SL  WHERE -        ,         000000
00114     18*          1          36H  TL-TEMPERATURE                      ,         000000
00114     19*          2          36H CPL-CONSTANT PRESSURE SPECIFIC HEAT,          000000
00114     20*          3          36H  HL-ENTHALPY                         ,         000000
00114     21*          4          36H  SL-ENTROPY                          /         000000
00114     22*      C                                                                 000000
00116     23*              NLTSP=0                                                   000000
00117     24*              CALL PAGI                                                 000000
00120     25*              CALL CHRSIZ(3;                                            000002
00121     26*       10     CALL GOUT(INLIMN,56)                                      000006
00122     27*              CALL RDATAI(1,NLTSP,$10)                                  000011
00122     28*      C                                                                 000011
00122     29*      C            LOOP FOR EACH SPECIES                                000011
00123     30*                   DO 60 I=1,NLTSP                                      000016
00126     31*       20          CALL GOUT(ISNMN,17)                                  000026
00127     32*                   CALL RDCHAR(RDUM,2,-1,$20)                           000031
00130     33*                   DECODE(100,RDUM) (SUBLT(I,J),J=1,3)                  000037
00136     34*       30          CALL GOUT(ITMPMN,42)                                 000051
00137     35*                   CALL RDATAI(1,NT,$30)                                000056
00140     36*                   IF(NT.LT.1 .OR. NT.GT.3) GO TO 30                    000064
00142     37*                   ILSP(I)=0                                            000102
00142     38*      C                                                                 000102
00142     39*      C                 LOOP FOR EACH TEMPERATURE                       000102
00143     40*                        DO 50 K=1,NT                                    000103
00146     41*                        DO 45 J=1,5                                     000113
00151     42*                        CALL GOUT(IMN(J,1),36)                          000113
00152     43*       45               CONTINUE                                        000124
00154     44*       46               CONTINUE                                        000124
00155     45*                        DO 48 J=1,4                                     000124
00160     46*                        RDUM(J)=0.                                      000124
00161     47*       48               CONTINUE                                        000125
00163     48*                        CALL RDATAF(4,RDUM,$46)                         000125
00164     49*                        TL(I,K)=RDUM(1)                                 000132
00165     50*                        CPL(I,K)=RDUM(2)                                000134
00166     51*                        HL(I,K)=RDUM(3)                                 000136
00167     52*                        SL(I,K)=RDUM(4)                                 000140
00170     53*                        ILSP(I)=ILSP(I)+1                               000142
00171     54*                        CPL(I,K)=CPL(I,K)/RBAR                          000145
00172     55*                        HL(I,K)=HL(I,K)/(TL(I,K)*RBAR)                  000147
00173     56*                        SL(I,K)=SL(I,K)/RBAR                            000152
00174     57*       50               CONTINUE                                        000163
00174     58*      C                                                                 000163
00174     59*      C            END SPECIES LOOP                                     000163
00176     60*       60          CONTINUE                                             000163
00176     61*      C                                                                 000163
00200     62*              RETURN                                                    000163
00200     63*      C                                                                 000163
00201     64*      100     FORMAT(3A4)                                               000220
00201     65*      C                                                                 000220
00202     66*              END                                                       000220

    END OF COMPILATION:        NO DIAGNOSTICS.
```

```
LTCPHS                                                                                DATE 101580        PAGE     3
 @HDG,P       MAIN
```

```
@FOR,S    MAIN,MAIN
MSA  E3 -10/15/80-13:07:06 (30,)

    MAIN PROGRAM

    STORAGE USED: CODE(1) 001514; DATA(0) 000720; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003    CONSTS 000006
     0004    MOLCON 000010
     0005    POINTS 000335
     0006    SPECES 017106
     0007    MISC   001701
     0010    INDX   000041
     0011    PERF   000166
     0012    CCC    000003
     0013    CFUEL  000009
     0014    MIN2   000002

    EXTERNAL REFERENCES (BLOCK, NAME)

     0015    RDYES
     0016    MPSINT
     0017    PAGIT
     0020    CHRSIZ
     0021    GOUT
     0022    RDATAI
     0023    RREAD
     0024    COALCV
     0025    LTCPHS
     0026    ROCHAR
     0027    MDCODS
     0030    MOVABS
     0031    MOLDIT
     0032    REACT
     0033    SEARCH
     0034    THERMP
     0035    DETON
     0036    ROCKET
     0037    SHCK
     0040    MPSTRM
     0041    NINTR$
     0042    NWDU$
     0043    NIO2$
     0044    NERR2$
     0045    NRCW$
     0046    NRDU$
     0047    NIO3$
     0050    NIO1$
     0051    NRNL$
     0052    NWNL$
     0053    NWEF$
     0054    ALOG
     0055    NSTOP$
```

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MAIN                                                                                    DATE 101580        PAGE     2

  STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

  0000   000530 10F      0001   000406 108L     0001   000233 11L      0001   000601 11211L   0001   000536 1211L
  0001   000574 1212L    0001   000733 1215L    0001   001037 1205L    0001   000237 15L      0001   000021 1546
  0001   000414 181L     0001   000057 2L       0000   000537 20F      0001   000076 203L     0001   000444 205L
  0001   000452 206L     0000   000577 207F     0001   000505 208L     0000   000646 21F      0001   000513 210L
  0000   000615 211F     0001   000762 213L     0001   000777 214L     0001   000633 215L     0000   000551 22F
  0001   000403 25L      0001   001506 3L       0001   001446 301L     0001   001450 302L     0001   001046 304L
  0001   001122 307L     0001   001104 322L     0001   001153 323L     0001   000367 3276     0001   001211 333L
  0001   000437 3526     0001   000471 3676     0001   000243 34L      0000   000377 400F     0001   000540 4156
  0001   001363 432L     0000   000526 5F       0001   000705 5176     0001   000714 5226     0001   000740 5326
  0001   000756 544G     0001   001014 5716     0001   001050 6106     0001   001106 6256     0001   001130 6406
  0001   001267 7076     0001   001126 722L     0000   000637 724F     0001   001331 7246     0001   001217 745L
  0001   001404 7466     0001   001254 746L     0001   001341 748L     0001   001416 7516     0001   001430 7566
  0001   001452 790L     0001   001462 791L     0001   001476 800L     0001   000246 90L      0001   000277 97L
  0006 R 011052 A        0011   000150 AEAT     0007   000640 AM       0007   000705 AM1      0007   001135 ANUM
  0011   000133 APP      0003 R 000000 ATMN     0007   000004 ATOM     0004 I 000004 BLANK    0007   000514 BO
  0007 R 000545 BPR      0010 L 000016 CALCM    0013 R 000000 CF       0000   000000 COEF     0010   000001 CONVG
  0005   000032 CPR      0007   000706 CPR1     0007   000634 CPSUM    0007 I 000654 DATA     0006   010624 DELN
  0012   000002 DEMAND   0007   001560 DENS     0000 L 000244 DETN     0005   000064 DLVPT    0005   000047 DLVTP
  0006 R 004312 EN       0000 I 000000 END      0006 R 010150 ENLN     0007   001700 ENLSAV   0007 R 000000 ENN
  0007 R 001676 ENNL     0007   001677 ENSAVE   0006 I 010624 ENSERT   0007   001414 ENTH     0011 L 000165 EOL
  0007 R 000636 EQRAT    0000 L 000245 ERATIO   0000 L 000256 FA       0007   001445 FAZ      0000 L 000257 FIRST
  0007   001527 FOX      0000 L 000247 FPCT     0005   000101 GAMMAS   0004   000001 GAS      0003   000001 GMET
  0012   000000 GRAPH    0013   000001 HHVV     0010 L 000003 HP       0007   000642 HPP      0007   000637 HSUBO
  0005   000000 HSUM     0006   010376 HO       0000 I 000231 I        0010   000030 IC       0000 I 000262 ICARD
  0010 I 000000 IDEBUG   0004 I 000002 IE       0010   000015 IMAT     0000 I 000260 INAM     0000   000265 INPT2
  0000 I 000232 INSERT   0010 L 000023 IONS     0010   000021 IP       0010   000037 IOSAVE   0010 I 000016 IO1
  0000 I 000264 IST      0010   000005 ISV      0010 I 000034 IT       0006 I 010266 IUSE     0004 I 000003 IZ
  0000 I 000263 J        0010   000026 JLIQ     0012 I 000001 JOUT     0010   000025 JSOL     0010   000031 JS1
  0010   000014 KMAT     0010 I 000012 L        0007 I 000463 LLMT     0010   000040 LSAVE    0000 I 000233 MIT
  0007 R 001644 MIX      0000 I 000235 MLOW     0000 L 000250 MMHG     0004   000005 MOL      0010 L 000006 MOLES
  0007 I 000707 NAME     0010 I 000024 NC       0000 I 000236 NCO      0010 L 000022 NEWR     0010   000035 NFZ
  0000 I 000234 NMLT     0010 I 000017 NOF      0010 I 000020 NOMIT    0000 I 000003 NOMTS    0010 I 000007 NP
  0010   000011 NPT      0010 I 000027 NREAC    0010 I 000013 NS       0000 I 000261 NSERT    0000 I 000000 NSPP1
  0000 L 000251 NSQM     0010 I 000010 NT       0014 I 000000 N1       0014 I 000001 N2       0007 L 000635 OF
  0006 I 010150 OMIT     0004   000006 OX       0007 R 001644 OXF      0007 R 000635 OXFL     0005 R 000116 P
  0003 R 000002 PATM     0011   000000 PCP      0007   001363 PECWT    0013 R 000003 PER      0007   000633 PP
  0005   000217 PPP      0000 L 000252 PSIA     0003 R 000003 RBAR     0003   000004 RBR      0000 R 000242 RDUM
  0015 L 000000 RDYES    0000 I 000001 REAC     0007   000644 RH       0007 R 001611 RHOP     0000 L 000253 RKT
  0007   001612 RMW      0007   001476 RTEMP    0003   000005 RVR      0006   004064 S        0010 L 000033 SHOCK
  0006   016660 SLN      0007 R 000003 SO       0005   000251 SONVEL   0010 L 000004 SP       0013   000047 SPIN
  0005   000015 SSUM     0006 I 015364 SUR      0011   000101 SUBAR    0007 R 000001 SUMN     0011   000116 SUPAR
  0000 L 000254 SV       0007 R 000003 SQ       0005 R 000150 T        0006   016514 TEMP     0007 R 000632 THIGH
  0000 I 000002 THRM     0007   001643 TLN      0007 R 000630 TLOW     0007   000627 TM       0007 R 000631 TMID
  0005   000320 TOTM     0010 L 000002 TP       0007   000002 TT       0005   000266 TTT      0000 L 000255 TV
  0000 L 000256 UV       0005 R 000202 V        0011   000064 VACI     0005   000303 VLM      0007 R 000646 VMIN
  0011   000032 VMOC     0010 L 000032 VOL      0007 R 000650 VPLS     0013   000002 WCR      0005   000234 WM
  0007 R 000652 WP       0004   000007 ZERO


00100      1*     C  MAIN PROGRAM                                                     MAIN0002     000000
00100      2*     C                                                                                000000
00101      3*            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                  /CONSTS/     000000
```

```
00103     4*        COMMON /MOLCON/ END,GAS,IE,IZ,BLANK,MOL,OX,ZERO                     /MOLCON/   000001
00104     5*        COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                    000001
00104     6*       1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),              000001
00104     7*       2 ,VLM(13),TOTN(13)                                                             000001
00104     8*    C   COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),MO(150)                000001
00104     9*    C  1 ,DELN(150),A(15,150),SUB(150,1),IUSE(150),TEMP(50,2),SLM(150)                 000001
00105    10*        INCLUDE SPECPR                                                                 000001
00111    11*        COMMON /MISC/ ENN,SUMNN,TT,S0,ATOM(3,101),LLMT(25),BO(25),                     000001
00111    12*       1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                  000001
00111    13*       2              MSUBO,AM(2),MPP(2),RH(2),VMIN(2),VPLS(2),WP(2),       /MISC/     000001
00111    14*       3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(13,6),PECWT(25),               000001
00111    15*       4              ENIM(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RMOP,                000001
00111    16*       5              RMW(25),TLN,OXF(26),ENML,ENSAVE,ENLSAV                           000001
00112    17*        COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,       /INDX/     000001
00112    18*       1              NMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,    /INDX/     000001
00112    19*       2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE      /INDX/     000001
00113    20*        COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),         /PERF/     000001
00113    21*       1              SUPAR(13),APP(13),AEAT(13),EQL                        /PERF/     000001
00113    22*    C                                                                                  000001
00114    23*           COMMON /CCC/ GRAPH,JOUT,DEMAND                                              000001
00115    24*        COMMON /CFUEL/CF,MMVV,WCP,PER                                                  000001
00116    25*        COMMON /N1N2/N1,N2                                                             000001
00117    26*        INTEGER BLANK,DATA,END,ENSERT,OMIT,REAC,SUB,THRM                               000001
00120    27*        DIMENSION NOMTS(150)                                                           000001
00121    28*        DATA (NOMTS(I),I=1,41)/                                                        000001
00121    29*       X'AL(C','       ',','AL(L','        ','      ',                                 000001
00121    30*       X'ALCL ','2     ',','ALN(','S)      ','      ',                                 000001
00121    31*       X'ALN ','       ',','C    ','        ','      ',                                 000001
00121    32*       X'C3  ','       ',','C4   ','        ','      ',                                 000001
00121    33*       X'C5  ','       ',                                                              000001
00121    34*       X'H2O(','S)     ',                                                              000001
00121    35*       X'O3  ','       ',','SI   ','        ','      ',                                 000001
00121    36*       X'SIC ','       ',','SIC2','        ','      ',                                 000001
00121    37*       X'SI(S','       ',','SI(L','        ','      ',                                 000001
00121    38*       X'SICL','       ',','SICL','2       ','      ',                                 000001
00121    39*       X'SICL','3      ',','SICL','4       ','      ',                                 000001
00121    40*       X'SIN ','       ',','SIN4','        ','      ',                                 000001
00121    41*       X'SIN ','       ',','SI2 ','        ','      ',                                 000001
00121    42*       X'SI2O','       ',','SI2N','        ','      ',                                 000001
00121    43*       X'SI3 ','       ',                                                              000001
00121    44*       X  /                                                                            000001
00123    45*        DATA INSERT,MIT,MMLT,REAC,THRM/4HINSE,4HOMIT,4HNAME,4HREAC,4HTHER/             000001
00131    46*        DATA MLOW/4HLOW /                                                              000001
00133    47*        DIMENSION ENSERT(3,3),NCO(4),OMIT(3,3)                                         000001
00134    48*        DIMENSION RDUM(2)                                                              000001
00135    49*        EQUIVALENCE (DELN,ENSERT),(ENLN,OMIT),(MIX,OXF),(OF,OXFL),(SO,SO)              000001
00136    50*        LOGICAL CALCH,DETN,EQL,ERATIO,FA,FPCT,HP,IONS,MMHG,MOLES,NEWR,                 000001
00136    51*       1        NSQM,OF,PSIA,RKT,SHOCK,SP,SV,TP,TV,UV,VOL                              000001
00136    52*    C                                                                                  000001
00137    53*           LOGICAL ROVFS,FIRST                                                         000001
00137    54*    C                                                                                  000001
00140    55*        REAL MIX(26)                                                                   000001
00140    56*    C                                                                                  000001
00141    57*        NAMELIST /INPT2/ DETN,ERATIO,FA,FPCT,HP,IDEBUG,IONS,MIX,MMHG,NSQM, /INPT2/     000001
00141    58*       1                 OF,P,PSIA,RKT,SO,SHOCK,SO,SP,SV,T,TP,TV,UV,V      /INPT2/     000001
00142    59*        DATA INAM/10/                                                                  000001
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 00142     60*     C                                                                000001
 00144     61*              FIRST=.TRUE.                                            000001
 00145     62*                 CALL MPSINT                                          000003
 00146     63*              CF=-1.0                                                 000005
 00147     64*              N1=0                                                    000007
 00150     65*              N2=0                                                    000010
 00151     66*            1 WRITE(JOUT,400)                                         000011
 00153     67*              DO 300 I=1,6                                            000021
 00156     68*              MIX(I) = 0.0                                            000021
 00157     69*              P(I)= 0.                                  ODE    115    000021
 00160     70*              T(I)= 0.                                  ODE    116    000022
 00161     71*          300 V(I) = 0.0                                              000023
 00163     72*              TP = .FALSE.                              ODE    123    000025
 00164     73*              HP=.TRUE.                                               000026
 00165     74*              TV = .FALSE.                                            000030
 00166     75*              UV = .FALSE.                                            000031
 00167     76*              SV = .FALSE.                                            000032
 00170     77*              RKI=.FALSE.                                             000033
 00171     78*              SO=0.0                                                  000034
 00172     79*              SP=.FALSE.                                              000035
 00173     80*              SHOCK = .FALSE.                           ODE    129    000036
 00174     81*              DETN = .FALSE.                            ODE    130    000037
 00175     82*              MMHG   = .FALSE.                          ODE    133    000040
 00176     83*              PSIA = .TRUE.                                           000041
 00177     84*              NSOM = .FALSE.                                          000043
 00200     85*              IONS = .FALSE.                                          000044
 00201     86*              IDEBUG = 0                                              000045
 00202     87*              FA = .FALSE.                                            000046
 00203     88*              OF = .TRUE.                                             000047
 00204     89*              ERATIO = .FALSE.                                        000051
 00205     90*              FPCT = .FALSE.                                          000052
 00206     91*              EQL = .TRUE.                              ODE    145    000053
 00207     92*              NEWR = .FALSE.                            MAIN0022      000055
 00210     93*          400 FORMAT(1H1)                               MAIN0025      000057
 00211     94*            2 CONTINUE                                                000057
 00212     95*              NREAC=0                                                 000057
 00213     96*              NSERT=0                                                 000057
 00214     97*              NOMIT=0                                                 000060
 00215     98*                 CALL PAGIT                                           000061
 00216     99*                 JOUT=6                                               000063
 00217    100*                 IF(RDYES('TYPE  YES  FOR PRINT TO PRINT FILE',35)) JOUT=31   000065
 00221    101*      203        CONTINUE                                             000075
 00222    102*                 CALL PAGIT                                           000075
 00223    103*                 CALL CHRSIZ(1)                                       000076
 00224    104*                 CALL GOUT('LEWIS CHEMICAL EQUILIBRIUM PROGRAM',34)   000101
 00225    105*                 CALL GOUT(' ',1)                                     000105
 00226    106*                 CALL GOUT('          MAIN MENU',19)                  000111
 00227    107*                 CALL GOUT(' ',1)                                     000115
 00230    108*                 CALL GOUT(' 1 - INSERT THERMODYNAMICS DATA',31)      000121
 00231    109*                 CALL GOUT(' 2 - INSERT LOW TEMP EXTENSION THERMO DATA',42)   000125
 00232    110*                 CALL GOUT(' 3 - INSERT OR EDIT REACTANTS',29)        000131
 00233    111*                 CALL GOUT(' 4 - OMIT SPECIES FROM THERMO DATA',34)   000135
 00234    112*                 CALL GOUT(' 5 - INSERT CONDENSED SPECIES',29)        000141
 00235    113*                 CALL GOUT(' 6 - INSERT OR EDIT NAMELIST',28)         000145
 00236    114*                 CALL GOUT(' 7 - START PROGRAM CALCULATION',30)       000151
 00237    115*                 CALL GOUT(' 8 - INSERT OR EDIT COAL DATA',29)        000155
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00240     116*            CALL GOUT(' RETURN - TERMINATE PROGRAM',27)          000161
00241     117*              ICARD=0                                            000165
00242     118*          CALL CHRSIZ(4)                                         000166
00243     119*            CALL RDATA7(1,ICARD,$203)                            000171
00244     120*             IF(ICARD.EQ.0) GO TO 3                              000176
00246     121*          IF (ICARD.LT.0.OR.ICARD.GT.8) GO TO 203                000200
00250     122*          GO TO (90,39,11,205,108,210,215,15),ICARD              000215
00250     123*      C                                                          000215
00250     124*      C        CALL SUBROUTINE TO READ REACTANT CARDS            000215
00251     125*        11 CALL RREAD(FIRST)                                     000233
00252     126*          GO TO 203                                              000235
00252     127*      C   COAL COMPOSITION INPUT                                 000235
00253     128*        15 CALL COALCV(FIRST)                                    000237
00254     129*          GO TO 203                                              000241
00254     130*      C                                                          000241
00254     131*      C   READ LOW TEMPERATURE EXTENSION THERMO DATA             000241
00255     132*       39 CALL LTCPHS                                            000243
00256     133*          GO TO 203                                              000244
00256     134*      C                                                          000244
00256     135*      C   READ THERMO DATA FROM CARDS AND STORE ON  TAPE 4       000244
00257     136*        90 NEWR = .TRUE.                                         000246
00260     137*          REWIND 4                                               000247
00261     138*               CALL GOUT('ADD THERMO DATA HERE',20)              000252
00262     139*          READ(5,5) TLOW,TMID,THIGH                              000256
00267     140*         5 FORMAT (3F10.3)                                       000266
00270     141*          WRITE (4,5) TLOW,TMID,THIGH                            000266
00275     142*        97 READ (5,10) (DATA(I),I=1,16),NCD(1)                   000277
00301     143*        10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)           000310
00302     144*          IF(DATA(1).EQ.BLANK) DATA(1)=END                       000310
00304     145*          WRITE (4,10) (DATA(I),I=1,16)                          000315
00307     146*          IF(DATA(1).EQ.END)  GO TO 203                          000325
00311     147*          READ (5,20) (DATA(I), I = 1,5),NCD(2),(DATA(J), J = 6,10),NCD(3),    000330
00311     148*         1                (DATA(I), I = 11,14),NCD(4)            000330
00321     149*        20 FORMAT(5E15.8,I5/5E15.8,I5/4E15.8,I20)                000354
00322     150*          WRITE (4,21) (DATA(I), I = 1,14)                       000354
00325     151*        21 FORMAT(5E15.8/5E15.8/4E15.8)                          000367
00326     152*          DO 25  I=1,4                                           000367
00331     153*          IF(NCD(I).EQ.I)  GO TO 25                              000367
00333     154*          WRITE(JOUT,22) (DATA(J),J=1,3)                         000372
00336     155*        22 FORMAT(28HOERROR IN ORDER OF CARDS FOR ,3A4)          000404
00337     156*        25 CONTINUE                                              000404
00341     157*          GO TO 97                                               000404
00341     158*      C                                                          000404
00341     159*      C    CHECK INSERT CARDS                                    000404
00342     160*       108      CONTINUE                                         000406
00343     161*                CALL PAGIT                                       000406
00344     162*                CALL GOUT('TYPE SPECIES TO INSERT(1 PER LINE)',34)     000407
00345     163*      181       CONTINUE                                         000414
00346     164*                CALL RDCHAR(RDUM,2,-1,$203)                      000414
00347     165*                NSERT=NSERT+1                                    000421
00350     166*                DECODE (207,RDUM) (ENSERT(I,NSERT),I=1,3)        000424
00356     167*                GO TO 181                                        000442
00356     168*      C                                                          000442
00356     169*      C     CHECK OMIT CARDS                                     000442
00357     170*       205      CONTINUE                                         000444
00360     171*                CALL PAGIT                                       000444
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00361    172*              CALL GOUT('TYPE SPECIES TO OMIT FROM THERMO DATA',37)            000445
00362    173*      206     CONTINUE                                                         000452
00363    174*              CALL RDCHAR(RDUM,2,-1,$208)                                      000452
00364    175*              NOMIT=NOMIT+1                                                    000457
00365    176*              DECODE (207,RDUM) (OMIT(I,NOMIT),I=1,3)                          000462
00373    177*      207     FORMAT(3A4)                                                      000503
00374    178*              GO TO 206                                                        000503
00375    179*        208 CONTINUE                                           MAIN0062        000505
00376    180*            NEWR= .TRUE.                                                       000505
00377    181*            REWIND 4                                                           000506
00400    182*            GO TO 203                                          MAIN0063        000511
00400    183*      C                                                                        000511
00400    184*      C     BEGIN NAMELIST INPT2                               MAIN0065        000511
00401    185*        210 CALL PAGIT                                                         000513
00402    186*            IF (.NOT.RDYES('TYPE YES FOR PRINT INPT2 NAMELIST',35)) GO TO 1211 000514
00402    187*      C     ACCESS THE ORIGINAL NAMELIST FROM PREVIOUS RUN                     000514
00404    188*            REWIND INAM                                                        000521
00405    189*            READ (INAM,INPT2)                                                  000524
00410    190*            WRITE (6,INPT2)                                                    000530
00413    191*            GO TO 1212                                                         000534
00413    192*      C     RESET ALL PARTS OF NAMELIST                                        000534
00414    193*       1211 DO 1210 I=1,26                                                     000540
00417    194*            MIX(I)=0                                                           000540
00420    195*            P(I)=0                                                             000540
00421    196*            T(I)=0                                                             000541
00422    197*       1210 V(I)=0                                                             000542
00424    198*            TP=.FALSE.                                                         000544
00425    199*            HP=.TRUE.                                                          000545
00426    200*            TV=.FALSE.                                                         000547
00427    201*            UV=.FALSE.                                                         000550
00430    202*            SV=.FALSE.                                                         000551
00431    203*            RKT=.FALSE.                                                        000552
00432    204*            SO=0.0                                                             000553
00433    205*            SP=.FALSE.                                                         000554
00434    206*            SHOCK=.FALSE.                                                      000555
00435    207*            DETN=.FALSE.                                                       000556
00436    208*            MMHG=.FALSE.                                                       000557
00437    209*            PSIA=.TRUE.                                                        000560
00440    210*            NSOM=.FALSE.                                                       000562
00441    211*            IONS=.FALSE.                                                       000563
00442    212*            IDEBUG=0                                                           000564
00443    213*            FA=.FALSE.                                                         000565
00444    214*            OF=.TRUE.                                                          000566
00445    215*            ERATIO=.FALSE.                                                     000570
00446    216*            FPCT=.FALSE.                                                       000571
00447    217*            GO TO 11211                                                        000572
00450    218*       1212 IF (.NOT.RDYES('TYPE YES TO CHANGE NAMELIST',27))                  000574
00450    219*          X    GO TO 203                                                       000574
00452    220*      11211 WRITE (6,211)                                                      000601
00454    221*      211      FORMAT(' BEGIN NAMELIST INPT2 INPUT')                           000605
00455    222*       2211 CONTINUE                                                           000605
00456    223*            READ(5,INPT2)                                      MAIN0086        000605
00456    224*      C     STORE NAMELIST                                                     000605
00461    225*            REWIND INAM                                                        000611
00462    226*            WRITE (INAM,INPT2)                                                 000614
00465    227*            ENDFILE INAM                                                       000620
```

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00466     228*           CALL MOVABS(800,50)                                               000623
00467     229*           CALL HOLDIT                                                       000627
00470     230*           GO TO 203                                                         000631
00471     231*       215 CONTINUE                                                          000633
00472     232*           FIRST=.FALSE.                                                     000633
00473     233*           CALL PAGIT                                                        000633
00474     234*           CALL GOUT(' ',1)                                                  000635
00475     235*           REWIND INAM                                                       000641
00476     236*           READ (INAM,INPT2)                                                 000644
00501     237*           WRITE (6,INPT2)                                                   000650
00504     238*           CALL MOVABS(500,50)                                               000654
00505     239*           CALL HOLDIT                                                       000660
00506     240*           CALL PAGIT                                                        000662
00507     241*           CALL GOUT(' ',1)                                                  000664
00510     242*           CALL REACT                                                        000670
00511     243*           IF (CF) 1215,,                                                    000672
00514     244*           IF (.NOT.ROYES('TYPE YES FOR SPECIAL OMITS FOR COAL DATA',40))    000675
00514     245*          X  GO TO 1215                                                      000675
00516     246*           DO 12 I=1,27                                                      000706
00521     247*           DO 12 J=1,3                                                       000714
00524     248*        12 OMIT(J,NOMIT+I)=NOMTS(I,3-3+J)                                    000721
00527     249*           NOMIT=NOMIT+27                                                    000727
00530     250*      1215 CALCH=.FALSE.                                                     000733
00531     251*           DO 755 I=1,NREAC                                                  000733
00534     252*           IF (NAME(I,6).EQ.IZ) CALCH=.TRUE.                                 000740
00536     253*       755 CONTINUE                                                          000746
00540     254*           IF (ERATIO) GO TO 213                                             000746
00542     255*           IF (CF) 213,,                                                     000750
00545     256*           DO 212 I=1,26                                                     000756
00550     257*       212 MIX(I)=MIX(I)*CF                                                  000756
00552     258*       213 IF (PER-1.0) ,214,                                                000762
00555     259*           NSERT=NSERT+1                                                     000764
00556     260*           ENSERT(1,NSERT)='IC(S'                                            000770
00557     261*           ENSERT(2,NSERT)=')    '                                           000772
00560     262*           ENSERT(3,NSERT)='     '                                           000774
00561     263*       214 CONTINUE                                                          000777
00562     264*           RHOP=0.                                                           000777
00563     265*           VOL=.FALSE.                                                       000777
00564     266*           NT=1                                                              001000
00565     267*           IF(.NOT.TV.AND..NOT.UV.AND..NOT.SV)  GO TO 304                    001002
00567     268*           VOL = .TRUE.                                                      001007
00570     269*           DO 1304  I=1,26                                                   001014
00573     270*           IF (P(I) .GT. 0.0)  P(I) = 1.0/P(I)                               001014
00575     271*           IF (V(I) .GT. 0.0)  P(I) = V(I)                                   001022
00577     272*           IF (P(I) .LE. 0.0)  GO TO 1305                                    001027
00601     273*      1304 NP = I                                                            001032
00603     274*      1305 TP = TV                                                           001037
00604     275*           HP = UV                                                           001040
00605     276*           SP = SV                                                           001042
00606     277*           GO TO 322                                                         001044
00607     278*       304 DO 305  I=1,26                                                    001050
00612     279*           IF (P(I) .LE. 0.0)  GO TO 322                                     001050
00614     280*           NP = I                                                 MAIN0090   001053
00615     281*           IF (MMHG) P(NP) = P(NP)/760.                                      001057
00617     282*           IF (PSIA)  P(NP) = P(NP)/PATM                                     001065
00621     283*       305 IF (NSOM)  P(NP) = P(NP)/ATMN                                     001073
```

```
00624    284*      322 DO 307 IT = 1,26                                                          001106
00627    285*          IF (T(IT) .LE. 0.0)  GO TO 722                                            001106
00631    286*          IF (CF+1.0) ,307,                                                         001111
00634    287*          T(IT)=(T(IT)-32.)/1.8+273.15                                              001114
00635    288*      307 NT = IT                                                                   001122
00637    289*      722 DO 625 IST = 1,26                                                         001130
00642    290*          IF (MIX(IST) .GT. 0.0)  GO TO 323                                         001130
00644    291*          IF(IST.NE.1) GO TO 745                                                    001133
00646    292*          WRITE(JOUT,724)                                                           001136
00650    293*      724 FORMAT (//5X,40HNO INPT2 VALUE GIVEN FOR FA, FPCT, OR OF//)               001143
00651    294*          IF (WP(2) .GT. 0.0)  OXFL = WP(1)/WP(2)                                   001143
00653    295*          GO TO 333                                                                 001151
00654    296*      323 OXFL=MIX(IST)                                                             001153
00655    297*          IF(FA) OXFL =1./   MIX(IST)                                               001154
00657    298*          IF(FPCT) OXFL =(100.-   MIX(IST))/   MIX(IST)                             001161
00661    299*          IF(.NOT.ERATIO)  GO TO 333                                                001167
00663    300*          EQRAT = MIX(IST)                                                          001171
00664    301*          IF(EQRAT.EQ.1.)  EQRAT = 1.000005                                         001173
00666    302*          OXFL  = (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))                  001200
00667    303*      333 OXF(IST) = OXFL                                                           001211
00670    304*      625 NOF = IST                                                                 001212
00672    305*      745 IF (.NOT. IONS .OR. LLMT(L) .EQ. IE)  GO TO 746                           001217
00674    306*          L = L+1                                                                   001227
00675    307*          IF(LLMT(L).NE.IE)  NEWR=.TRUE.                                            001232
00677    308*          REWIND 4                                                                  001242
00700    309*          LLMT(L) = IE                                                              001245
00701    310*          BOP(L,1) = 0.                                                             001250
00702    311*          BOP(L,2) = 0.                                                             001251
00703    312*          GO TO 748                                                                 001252
00704    313*      746 IF(LLMT(L).NE.IE)  GO TO 748                                              001254
00706    314*          DO 747  J=1,NS                                                            001257
00711    315*      747 IF (A(L,J) .NE. 0.0)  IUSE(J) = - 10000                                   001267
00714    316*          L = L-1                                                                   001275
00715    317*      748 IF(NEWR)  CALL SEARCH                                                     001301
00715    318*    C     INITIAL ESTIMATES                                                         001301
00717    319*          SO = SO/RBAR                                                              001304
00720    320*          ENN = .1                                                                  001307
00721    321*          ENNL = -2.3025851                                                         001311
00722    322*          SUMN = ENN                                                 MAIN0141       001313
00723    323*          DO 432 J=1,NS                                              MAIN0145       001331
00726    324*          IF(IUSE(J).GT.0)  IUSE(J)=-IUSE(J)                                        001331
00730    325*          IF(IUSE(J).EQ.-10000.AND.IONS)  IUSE(J) = 0                               001335
00732    326*          EN(J,1) = 0.                                                              001346
00733    327*          ENLN(J) = 0.                                                              001347
00734    328*          IF (IUSE(J).NE.0)  GO TO 432                                              001350
00736    329*          EN(J,1) = ENN/(NS - NC)                                                   001352
00737    330*          ENLN(J) = ALOG(EN(J,1))                                                   001354
00740    331*      432 CONTINUE                                                                  001364
00742    332*          IQ1= L+1                                                                  001364
00743    333*          IF (NC.EQ.0.OR.NSERT.EQ.0) GO TO 790                                      001367
00745    334*          DO 302 I=1,NSERT                                                          001377
00750    335*          DO 301 J=1,NS                                                             001416
00753    336*          IF(IUSE(J).EQ.0) GO TO 301                                                001421
00755    337*          DO 299 IST = 1,3                                                          001430
00760    338*      299 IF (SUB(J,IST) .NE. ENSERT(IST,I))  GO TO 301                             001430
00763    339*          IQ1= IQ1+1                                                                001437
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00764     340*           IUSE(J)= -IUSE(J)                                                001442
00765     341*           GO TO 302                                                        001444
00766     342*       301 CONTINUE                                                         001452
00770     343*       302 CONTINUE                                                         001452
00772     344*       790 IF (.NOT. TP .AND. .NOT. HP .AND. .NOT. SP)  GO TO 791           001452
00774     345*           CALL THERMP                                                      001456
00775     346*           GO TO 800                                                        001460
00776     347*       791 IF (DETN)  CALL DETON                                            001462
01000     348*           IF(RKT) CALL ROCKET                                              001465
01002     349*           IF(SHOCK)  CALL SHCK                                             001471
01004     350*       800 NSERT = 0                                                        001476
01005     351*           CALL MOVARS(SDD,SD)                                              001476
01006     352*           CALL HOLDIT                                                      001502
01007     353*           GO TO 2                                                          001504
01010     354*         3     CONTINUE                                                     001506
01011     355*               CALL MPSTRM                                                  001506
01012     356*               STOP                                                         001507
01013     357*           END                                             MAIN0153         001513

      END OF COMPILATION:        NO  DIAGNOSTICS.

   2H06,P      MATRIX
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MATRIX                                                                                                      DATE 101580        PAGE     1

@FOR,S    MATRIX,MATRIX
HSA E3 -10/15/80-13:07:13 (11,)

SUBROUTINE MATRIX     ENTRY POINT 001063

STORAGE USED: CODE(1) 001107; DATA(0) 000116; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003   POINTS 000335
0004   SPECES 017106
0005   MISC   001701
0006   DOUBLE 001560
0007   INDX   000041

EXTERNAL REFERENCES (BLOCK, NAME)

0010   NERR3$

STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001     000102 124G       0001     000103 127G       0001     000126 140G       0001     000215 154G       0001     000244 161G
0001     000672 175L       0001     000677 185L       0001     000453 217G       0001     001011 230L       0001     000567 244G
0001     000606 247G       0001     000623 257G       0001     001026 260L       0001     000757 303G       0001     001023 317G
0001     000276 55L        0001     000346 59L        0001     000372 62L        0001     000376 64L        0001     000511 65L
0001     000405 70L        0004 R   011052 A          0005     000690 AM         0005     000708 AM1        0005     001138 ANUM
0005     000004 ATOM       0005 R   000514 BO         0005     000545 BOP        0007     000036 CALCH      0004     000000 COEF
0007 L   000001 CONVG      0003     000032 CPR        0005     000706 CPR1       0005 R   000634 CPSUM      0005     000654 DATA
0004     010624 DELN       0005     001560 DENS       0003     000064 DLVPT      0003     000047 DLVTP      0004 R   004312 EN
0000 R   000013 ENERGY     0004 R   010150 ENLN       0005     001700 ENLSAV     0005 R   000000 ENN        0005     001676 ENNL
0005     001677 ENSAVE     0005     001414 ENTH       0005     000636 EQRAT      0000 R   000010 F          0005     001445 FAZ
0005     001527 FOX        0006 D   000000 G          0003     000101 GAMMAS     0007 L   000003 HP         0005     000642 HPP
0005 R   0006[illegible]7 HSUBO      0003 R   000000 HSUM       0004 R   010376 HO         0000 I   000003 I          0007     000030 IC
0007     0000[illegible] IDEBUG     0007 I   000015 IMAT       0000     000023 INJPS      0007     000023 IONS       0007     000021 IP
0007     0000[illegible] IOSAVE     0007 I   000016 IQ1        0000 I   000001 IQ2        0000 I   000002 IQ3        0007     000005 ISV
0007     000034 IT         0004 I   016266 IUSE       0000 I   000007 J          0007     000026 JLIQ       0007     000025 JSOL
0007     000031 JS1        0000 I   000004 K          0000 I   000006 KK         0007 I   000014 KMAT       0007 I   000012 L
0005     000463 LLMT       0007     000040 LSAVE      0007     000006 MOLES      0005     000707 NAME       0007     000024 NC
0007     000022 NEWR       0007     000035 NFZ        0007     000017 NOF        0007     000020 NOMIT      0007     000007 NP
0007 I   000011 NPT        0007     000027 NREAC      0007 I   000013 NS         0000 I   000000 NSPP1      0007     000010 NT
0005     000635 OF         0005     001644 OXF        0003     000116 P          0005     001363 PECWT      0005     000633 PP
0003     000217 PPP        0005     000644 RH         0005     001611 RHOP       0005     001612 RMW        0005     001476 RTEMP
0004 R   004064 S          0007     000033 SHOCK      0004     016660 SLN        0003     000251 SONVEL     0007 L   000004 SP
0000 R   00001[illegible] SS         0000 R   000005 SSS        0003     000015 SSUM       0004     015364 SUB        0005 R   000001 SUMN
0005 R   000003 SO         0003     000150 T          0004     016514 TEMP       0000 R   000012 TERM1      0005     000632 THIGH
0005     001643 TLN        0005     000630 TLOW       0005 R   000627 TM         0005     000631 TMID       0003     000320 TOTN
0007 L   000002 TP         0005 R   000002 TT         0003     000266 TTT        0003     000202 V          0003     000303 VLM
0005     000646 VMIN       0007 L   000032 VOL        0005     000650 VPLS       0003     000234 WM         0005     000652 WP
0006 D   001510 X
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00101     1*           SUBROUTINE MATRIX                                                       MATX0001    000030
00101     2*     C                                                                                         000030
00103     3*           COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                         000030
00103     4*           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                   000030
00103     5*           2 ,VLM(13),TOIN(13)                                                                 000030
00103     6*     C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                     000030
00103     7*     C     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                     000030
00104     8*           INCLUDE SPECPK                                                                      000030
00110     9*           COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                           000030
00110    10*           1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,L,SUM,OF,EQRAT,                      000030
00110    11*           2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),         /MISC/       000030
00110    12*           3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),                   000030
00110    13*           4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,                    000030
00110    14*           5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                               000030
00111    15*           COMMON /DOUBLE/ G(20,21), X(20)                                         MATX0012    000030
00112    16*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,           /INDX/      000030
00112    17*           1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JL,IO,      /INDX/      000030
00112    18*           2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE         /INDX/      000030
00112    19*     C                                                                                         000030
00113    20*           DOUBLE PRECISION G,X                                                                000030
00114    21*           LOGICAL CONVG,HP,SP,TP,VOL                                                          000030
00114    22*     C                                                                                         000030
00115    23*           IQ2 = IQ1 + 1                                                                       000030
00116    24*           IQ3 = IQ2 + 1                                                                       000033
00117    25*           KMAT = IQ3                                                              MATX0018    000035
00120    26*           IF(.NOT.CONVG.AND.TP) KMAT = IQ2                                        MATX0019    000036
00122    27*           IMAT = KMAT - 1                                                         MATX0020    000046
00122    28*     C     CLEAR MATRIX STORAGES TO ZERO                                           MATX0022    000046
00123    29*           DO 211 I=1,IMAT                                                                     000057
00126    30*           DO 211 K=1,KMAT                                                                     000103
00131    31*       211 G(I,K) = 0.000                                                                      000103
00134    32*           SSS = 0.                                                                            000111
00135    33*           HSUM(NPT) = 0.                                                                      000112
00135    34*     C     BEGIN SET UP OF ITERATION MATRIX                                        MATX0028    000112
00136    35*           KK = L                                                                              000114
00137    36*           DO 65  J=1,NS                                                           MATX0031    000127
00142    37*           IF(IUSE(J).LT.0)  GO TO 65                                                          000141
00144    38*           IF(IUSE(J).GT.0)  GO TO 70                                                          000145
00146    39*           F = (HO(J)-S(J)+ENLN(J)+TM)*EN(J,NPT)                                               000150
00147    40*           SS = HO(J)*EN(J,NPT) - F                                                            000157
00150    41*           TERM1 = HO(J)*EN(J,NPT)                                                             000161
00151    42*           IF (KMAT .EQ. IQ2) TERM1 = F                                            MATX0037    000163
00153    43*           DO 55 I = 1, L                                                          MATX0038    000174
00153    44*     C     CALCULATE THE ELEMENTS  R(I,K)                                          MATX0040    000174
00156    45*           IF (A(I,J) .EQ. 0.) GO TO 55                                            MATX0042    000232
00160    46*           DO 15  K=I, L                                                           MATX0044    000234
00163    47*        15 G(I,K) = G(I,K) + A(K,J)*A(I,J)*EN(J,NPT)                                           000244
00165    48*           G(I,IQ1) = G(I,IQ1) + A(I,J)*EN(J,NPT)                                              000251
00166    49*           G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1                                          MATX0048    000255
00167    50*           IF (CONVG .OR.TP) GO TO 55                                              MATX0049    000261
00171    51*           G(I,IQ3)= G(I,IQ3)+A(I,J)*F                                             MATX0050    000263
00172    52*           IF (SP) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS                                 MATX0051    000267
00174    53*        55 CONTINUE                                                                MATX0052    000305
00176    54*           IF (KMAT .EQ. IQ2) GO TO 64                                             MATX0053    000305
00200    55*           IF(CONVG.OR.HP) GO TO 59                                                MATX0054    000310
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00202     56*           G(IQ2,IQ1) = G(IQ2,IQ1) + SS                          MATX0055   000323
00203     57*           G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*SS                        MATX0056   000326
00204     58*           G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - ENLN(J)-TM)*F         MATX0057   000334
00205     59*           GO TO 62                                              MATX0058   000344
00206     60*      59   G(IQ2,IQ2) = G(IQ2,IQ2) + HO(J)**2*EN(J,NPT)                     000346
00207     61*           IF (CONVG) GO TO 68                                   MATX0060   000362
00211     62*           G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*F                         MATX0061   000364
00212     63*      62   G(IQ1,IQ3)=G(IQ1,IQ3)+F                               MATX0062   000372
00213     64*      64   G(IQ1,IQ2)=G(IQ1,IQ2)+TERM1                           MATX0063   000376
00214     65*           GO TO 65                                                         000403
00214     66*     C     CONDENSED SPECIES                                                000403
00215     67*      70   KK = KK + 1                                                      000405
00216     68*           DO 75  I = 1,L                                                   000407
00221     69*           G(I,KK) = A(I,J)                                                 000453
00222     70*      75   G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)                         000454
00224     71*           G(KK,IQ2) = HO(J)                                                000462
00225     72*           G(KK,KMAT) = HO(J) - S(J)                                        000465
00226     73*           HSUM(NPT) = HSUM(NPT) + HO(J)*EN(J,NPT)                          000471
00227     74*           IF(.NOT.SP) GO TO 65                                             000477
00231     75*           SSS = SSS + S(J)*EN(J,NPT)                                       000501
00232     76*           G(IQ2,KK) = S(J)                                                 000505
00233     77*      68   CONTINUE                                              MATX0064   000520
00235     78*           SSS = SSS + G(IQ2,IQ1)                                           000520
00236     79*           HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)                               000527
00237     80*           G(IQ1,IQ1) = SUMN - ENN                                          000537
00237     81*     C     REFLECT SYMMETRIC PORTIONS OF THE MATRIX              MATX0066   000537
00240     82*           K = IQ1                                                          000543
00241     83*           IF (HP .OR. CONVG)  K = IQ2                                      000545
00243     84*           DO 102 I = 1,K                                                   000562
00246     85*           DO 102 J = I,K                                                   000604
00251     86*     102   G(J,I) = G(I,J)                                                  000606
00251     87*     C     COMPLETE THE RIGHT HAND SIDE                          MATX0074   000606
00254     88*           IF(CONVG)  GO TO 175                                  MATX0076   000612
00256     89*           DO 145 I=1,L                                          MATX0077   000623
00261     90*           X(I)=BO(I)-G(I,IQ1)                                              000623
00262     91*     145   G(I,KMAT) = G(I,KMAT) + X(I)                                     000625
00264     92*           G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN                    MATX0080   000630
00264     93*     C     COMPLETE ENERGY ROW AND TEMPERATURE COLUMN            MATX0082   000630
00265     94*           IF (KMAT .EQ. IQ2) GO TO 185                          MATX0084   000636
00267     95*           IF (SP)ENERGY = SO+ENN-SUMN - SSS                                000641
00271     96*           IF(HP)ENERGY=HSUBO/TT - HSUM(NPT)                                000656
00273     97*           G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY                                    000665
00274     98*     175   G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM                          MATX0088   000672
00275     99*     185   IF (.NOT. VOL .OR. CONVG)  RETURN                                000677
00275    100*     C     CONSTANT VOLUME MA RIX                                           000677
00277    101*           K = IQ1 - 1                                                      000704
00300    102*           IF(KMAT.EQ.IQ2) GO TO 230                                        000707
00302    103*           DO 220 I = 1,K                                                   000721
00305    104*           G(IQ1,I) = G(IQ2,I)-G(IQ1,I)                                     000757
00306    105*           G(I,IQ1) = G(I,IQ2)-G(I,IQ1)                                     000761
00307    106*     220   G(I,IQ2) = G(I,IQ3)                                              000764
00311    107*           G(IQ1,IQ1) = G(IQ2,IQ2)-G(IQ1,IQ2)-G(IQ2,IQ1)                    000767
00312    108*           G(IQ1,IQ2) = G(IQ2,IQ3)-G(IQ1,IQ3)                               000774
00313    109*           IF (HP)  G(IQ1,IQ2) = G(IQ1,IQ2) + ENN                           001001
00315    110*           GO TO 260                                                        001007
00316    111*     230   DO 240 I = 1,K                                                   001011
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     MATRIX                                                                                DATE 101580      PAGE

   00321     112*       240  G(I,IQ1) = G(I,IQ2)                                                  001023
   00323     113*        260 KMAT = IMAT                                                          001026
   00324     114*            IMAT = IMAT-1                                                        001027
   00325     115*            RETURN                                                               001031
   00326     116*            END                                                  MATX0090        001106

       END OF COMPILATION:       NO  DIAGNOSTICS.

   @HDG,P       OUT1
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@FOR,S    OUT1 OUT1
HSA  E3 -10/15/80-13:07:18 (15,)

    SUBROUTINE OUT1        ENTRY POINT 002156
               OUT2        ENTRY POINT 002161
               OUT3        ENTRY POINT 002164
               OUT4        ENTRY POINT 002167

    STORAGE USED: CODE(1) 002172; DATA(0) 000655; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003     CONSTS 000006
     0004     HOLCON 000010
     0005     POINTS 000335
     0006     SPECES 017106
     0007     MISC   001701
     0010     INDX   000041
     0011     PERF   000166
     0012     OUPT   000073
     0013     CCC    000003
     0014     CFUEL  000004

    EXTERNAL REFERENCES (BLOCK, NAME)

     0015     VARFMT
     0016     MOVABS
     0017     HOLDIT
     0020     PAGIT
     0021     NWDUS
     0022     NIO1$
     0023     NIO2$
     0024     NIO3$
     0025     SORT
     0026     NERR3$

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0000    000371 1F        0001    000034 10L       0001    001440 1014G     0001    001443 1020G     0001    001470 1034G
     0001    001477 1042G     0001    001510 1045G     0001    001520 1050G     0001    001564 1066G     0001    001573 1072G
     0001    001621 1107G     0001    001627 1115G     0001    001643 1124G     0001    001673 1135G     0001    001752 1153G
     0001    001760 1161G     0001    002030 1176G     0001    002042 1205G     0001    002054 1214G     0001    002066 1223G
     0001    002100 1232G     0001    002112 1241G     0001    001044 130L      0001    000025 154G      0001    001120 160L
     0001    000043 164G      0001    001144 170L      0001    001152 175L      0001    001221 177L      0001    001257 179L
     0001    001261 180L      0000    000377 2F        0000    000333 20F       0001    000112 200G      0001    001334 200L
     0001    001371 210L      0001    001373 211L      0000    000353 22F       0000    000310 240F      0001    000213 247G
     0001    000235 261G      0001    000276 277G      0000    000406 280F      0000    000422 290F      0001    000036 30L
     0000    000450 300F      0000    000452 310F      0001    000320 310G      0000    000416 320F      0001    000334 321G
     0001    000362 332G      0000    000412 340F      0001    000404 343G      0001    000420 350G      0001    000447 364G
     0001    000471 375G      0001    000501 403G      0001    000522 414G      0001    000544 425G      0001    000560 432G
     0001    000606 445G      0001    000065 45L       0001    000623 455G      0001    000647 471G      0000    000471 490F
     0000    000472 492F      0001    000217 50L       0001    001451 500L      0001    000670 502G      0000    000477 504F
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0001     001533 508L      0001     001536 510L      0001     000711 513G      0001     001604 514L      0001     000225 52L
0000     000504 520F      0001     000717 520G      0000     000511 524F      0001     000734 527G      0000     000517 532F
0001     000753 537F      0000     000525 542F      0000     000532 544F      0001     000763 545G      0000     000540 546F
0000     000546 548F      0000     000554 550F      0000     000562 552F      0001     001007 555G      0001     001075 610E
0001     001100 613G      0001     001106 620G      0001     001131 631G      0001     001140 636G      0001     000163 64L
0001     001157 650G      0001     001216 661G      0001     001247 673G      0001     001275 715G      0001     001307 720G
0001     001331 727G      0001     000342 74L       0001     001362 741G      0000     000405 &DF       0006     011052 A
0011     000150 AFAT      0007     000640 AM        0007     000705 AM1       0007 R   001136 ANUM      0011     000133 APP
0003 R   000000 ATMN      0007     000004 ATOM      0007     000514 BO        0007     000545 BOP       0010     000036 CALCH
0014 R   000000 CF        0000 R   000103 CMW       0006     000000 COEF      0000 R   000047 COF       0010     000001 CONVG
0005 R   000032 CPR       0007     000706 CPR1      0007     000634 CPSUM     0007     000654 DATA      0006     010624 DELN
0013     000002 DEMAND    0007 R   001560 DENS      0005 R   000064 DLVPT     0005 R   000043 DLVTP     0000 R   000236 DOL
0000 R   000167 EE        0006 R   004312 EN        0004     000000 END       0006     010150 ENLN      0007     001700 ENLSAV
0007     000000 ENN       0007     001676 ENNL      0007     001677 ENSAVE    0007 R   001414 ENTH      0011 L   000163 EOL
0007 R   000636 EQRAT     0012     000002 FA        0012 R   000003 FAP       0007 R   001445 FAZ       0012 R   000005 FB
0012     000006 FC        0012 R   000007 FCP       0012     000012 FCST      0012     000014 FCV       0012 R   000015 FG
0012     000017 FGE       0012     000020 FGV       0012 R   000021 FH        0000 R   000036 FHH       0012     000023 FI
0012     000026 FIY       0012 R   000027 FM        0012 R   000031 FMT       0012     000050 FN        0012 R   000052 FOUR
0007 I   001527 FOX       0012     000053 FP        0000 R   000046 FPC       0300 R   000032 FPP       0012 R   000054 FS
0000 R   000040 FSS       0012 R   000056 FSV       0012 R   000057 FT        0012 R   000061 FTK       0000 R   000034 FTR
0012 R   000063 FV        0012 R   000065 FVEL      0000 R   000001 FVLM      0012 R   000001 F13       0012     000000 F9X
0005 R   000101 GAMMAS    0004     000001 GAS       0003     000001 GMET      0013     000000 GRAPH     0000 R   000003 HEAD
0000 R   000221 HHVD      0000 R   000152 HHVS      0014 R   000001 HHVV      0010     000003 HP        0007     000642 HPP
0007     000637 HSUBO     0005 R   000000 HSUM      0006     010376 HO        0000 I   000042 I         0010     000030 IC
0010     000000 IDEBUG    0000 I   000261 IDG       0004     000002 IE        0000 I   000050 IFLAG     0000 I   000304 IJ
0010     000015 IMAT      0000 I   000253 INDX      0000     000624 INJPS     0010     000023 IONS      0010     000021 IP
0010     000037 IOSAVE    0010     000016 IO1       0006 I   015364 ISUB      0010     000005 ISV       0010     000034 IT
0004 I   016266 IUSE      0004     000003 IZ        0000 I   000045 J         0010     000026 JLIQ      0013 I   000001 JOUT
0010     000025 JSOL      0010     000031 JS1       0000 I   000043 K         0010     000014 KMAT      0004 I   000004 LANK
0000 R   000066 LHVD      0000 R   000051 LHVS      0007     000463 LLMT      0010     000040 LSAVE     0000 I   000305 L1
0000 I   000306 L3        0000 I   000307 L4        0004     000005 MOL       0010 L   000003 MOLES     0000 I   000014 MW
0007 I   000707 NAME      0010     000024 NC        0000 I   000044 NO        0010     000022 NEWR      0010     000035 NFZ
0010     000012 NLM       0010     000017 NOF       0010     000020 NOMIT     0010     000007 NP        0010 I   000011 NPT
0010 I   000027 NREAC     0010 I   000013 NS        0000 I   000000 NSPP1     0010     000010 NT        0007 R   000635 OF
0012 R   000067 ONE       0004 I   000006 OX        0007     001644 OXF       0005     000116 P         0003 R   000002 PATM
0011     000000 PCP       0007 R   001363 PECNT     0014 R   000003 PER       0007     000633 PP        0005 R   000217 PPP
0003 R   000003 RBAR      0003 R   000004 RBR       0007     000644 RH        0007 R   001611 RHOP      0007     001612 RHW
0007 R   001476 RTEMP     0003     000005 RVR       0006     004064 S         0010     000033 SHOCK     0006     016660 SLN
0005 R   000251 SONVEL    0010     000004 SP        0011     000047 SPIN      0005 R   000016 SSUM      0006 R   015364 SUB
0011     000101 SUBAR     0000 R   000303 SUM       0007     000001 SUMN      0011     000116 SUPAR     0007     000003 SO
0005     000150 T         0006     016514 TEMP      0007     000632 THIGH     0012     000070 THREE     0007     001643 TLN
0007     000630 TLOW      0007     000627 TM        0007     000631 THID      0005 R   000320 TOIN      0010     000002 TP
0007     000002 TT        0005 R   000266 TTT       0012 R   000071 TWO       0005 R   000202 V         0011     000064 VACI
0005 R   000303 VLM       0007     000646 VMIN      0011     000032 VMOC      0010 L   000032 VOL       0007     000650 VPLS
0014 R   000002 WCR       0005 R   000234 WM        0007     000652 WP        0000 R   000120 XDP       0000 R   000204 YDP
0004 R   000135 YDPS      0000 R   000020 YN        0000 R   000025 YX        0006 R   010376 Z         0004     000007 ZERO
0012     000072 ZEROF


00101      1*           SUBROUTINE OUT1                                                   OUTP0001     000000
00101      2*     C                                                                                    000000
00103      3*           COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                       /CONSTS/     000000
00104      4*           COMMON /MOLCON/ END,GAS,IE,IZ,LANK,MOL,OX,ZERO                    /MOLCON/     000000
00105      5*           COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                    000000
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00105     6.        1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)             000000
00105     7.        2 ,VLM(13), TOTN(13)                                                         000000
00105     8.   C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,3),ENLN(150),HO(150)              000000
00105     9.   C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150), TEMP(50,2),SLN(150)             000000
00106    10.         INCLUDE SPECPH                                                              000000
00112    11.         COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                   000000
00112    12.        1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,               000000
00112    13.        2              HSUMO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),      /MISC/   000000
00112    14.        3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),            000000
00112    15.        4              ENTH(25),FAZ(25),RTEMP(25),FOX(25), DENS(25),RHOP,            000000
00112    16.        5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                        000000
00113    17.         COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/   000000
00113    18.        1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,LIQ,    /INDX/   000000
00113    19.        2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE     /INDX/   000000
00114    20.         COMMON /PERF/ PCP(26),VMOC(13),SPIM(13), VACI(13),SUBAR(13),       /PERF/   000000
00114    21.        1              SUPAR(13),APP(13),AEAT(13),EQL                       /PERF/   000000
00115    22.         COMMON /OUPT/ FOX,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),    /OUPT/   000000
00115    23.        1              FGE,FGV,FH(2),FI(2),FIN(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/   000000
00115    24.        2              FP,FS(2),FSV,FT(2),FTN(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/   000000
00115    25.        3              TWO,ZEROF                                            /OUPT/   000000
00115    26.   C                                                                                 000000
00116    27.            COMMON /CCC/GRAPH,JOUT,DEMAND                                            000000
00117    28.         COMMON /CFUEL/CF,MHVV,WCR,PER                                               000000
00117    29.   C                                                                                 000000
00120    30.         DIMENSION FVLM(2),HEAD(9),MW(2,2),YN(5),YX(5),Z(10,3)                       000000
00121    31.         DIMENSION FPP(2),FTR(2),FHH(2),FSS(2)                                       000000
00122    32.         DATA (FPP(I),I=1,2)/'PRESS ','PSIA  '/                                      000000
00124    33.         DATA (FTR(I),I=1,2)/'TEMP D','EG F  '/                                      000000
00126    34.         DATA (FHH(I),I=1,2)/'ENTH B','TU/LB '/                                      000000
00130    35.         DATA (FSS(I),I=1,2)/'S BTU/','(LB-R)'/                                      000000
00132    36.         EQUIVALENCE (Z,HO)                                                          000000
00133    37.         INTEGER FOX,OX                                                              000000
00134    38.         LOGICAL EQL,MOLES,VOL                                                       000000
00134    39.   C                                                               OUTP0021          000000
00134    40.   C     HEAD = (1XA6,2X5(A2,F8.5,3X), 5X,F7.5,F13.3,4X,A1,F10.2,F9.4)               000000
00134    41.   C                                                                                 000000
00135    42.         DATA HEAD/6H(1XA6,,6H2X5(A2,6H,F8.4,,6H3X), 5,6HX,F7.5,6H,F13.3,            000000
00135    43.        1      6H,4X,A1,6H,F10.2,6H,F9.4)/,YN/6H2X1(A2,6H2X2(A2,6H2X3(A2,            000000
00135    44.        2      6H2X4(A2,6H2X5(A2/,YX/6H3X),57,6H3X),44,6H3X),31,6H3X),10,            000000
00135    45.        3 6H3X), 5/,MW/24HWT FRACTION     MOLES    /,FVLM/12HVOLUME CC/G /           000000
00135    46.   C                                                                                 000000
00143    47.         K = 1                                                                       000000
00144    48.         IF (MOLES)  K = 2                                                           000001
00146    49.         WRITE(JOUT,240) MW(1,K),MW(2,K)                                             000005
00152    50.     240 FORMAT (77X,2A6,30H ENTHALPY   STATE   TEMP   DENSITY/10X,                  000025
00152    51.        1         16HCHEMICAL FORMULA,65X,7HCAL/MOL,10X,6HDEG. K,3X,5HG/CM3)         000025
00153    52.         DO 60 K = 1,NREAC                                                           000028
00156    53.         IF (FOX(K) .NE. OX)  GO TO 10                                               000025
00160    54.         MD = 6HOXIDNT                                                               000030
00161    55.         GO TO 30                                                  OUT1 580          000032
00162    56.      10 MD = 6HFUEL                                                                 000034
00163    57.     30  DO 40 J=1,5                                               OUT1 610          000036
00166    58.      40 IF(ANUM(K,J) .LE. 0. .OR. NAME(K,J) .EQ. LANK)  GO TO 45                    000043
00171    59.         J=6                                                                         000062
00172    60.      45 J=J-1                                                                       000065
00173    61.         HEAD(2) = YN(J)                                                             000073
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00174                HEAD(4) = TX(J)                                                              000075
00175             60 WRITE(JOUT,HEAD) NO,(NAME(K,I),ANUM(K,I),I = 1,J),PECNT(K),                 000077
00175               1                    ENTH(K),FAZ(K),RTEMP(K),DENS(K)                          000077
00213                FPC = 100./(1.+OF)                                                           000126
00214                WRITE(JOUT,20) OF ,FPC,EQRAT,RHOP                                            000133
00222             20 FORMAT (1H0,15X,4HO/F=,F8.4,4X,13HPERCENT FUEL=,F8.4,4X,                    000144
00222               1 19HEQUIVALENCE RATIO= ,F7.4,4X,8HDENSITY=,F8.4)                             000144
00223                IF (CF+1.0) ,64,                                                             000144
00226                COF=OF/CF                                                                    000147
00227                WRITE (JOUT,22) COF,WCR,PER                                                  000152
00234             22 FORMAT (2X,'OXIDIZER/COAL=',F8.4,5X,'WATER/COAL=',F8.4,                      000163
00234               X    5X,'CARBON CONVERSION=',F8.4)                                            000163
00235             64 RETURN                                                                       000163
00235          C                                                                                  000163
00236                ENTRY OUT2                                                                   000165
00236          C     VOLUME                                                                       000165
00237                FMT(3) = ONE                                                                 000165
00240                IF(.NOT.VOL)  GO TO 50                                                       000167
00242                CALL VARFMT(VLM,NPT)                                                         000171
00243                WRITE(JOUT,FMT) FVLM,FB,(VLM(I), I = 1,NPT)                                  000175
00243          C   PRESSURE                                                         OUTP0038      000175
00253             50 IFLAG=0                                                                      000217
00254                IF (CF+1.0) ,52,                                                             000217
00257                IFLAG=1                                                                      000222
00260             52 DO 55 I=1,NPT                                                                000225
00263                IF (IFLAG.EQ.0) V(I)=ATMN*PPP(I)                                             000235
00265                IF (IFLAG.EQ.1) V(I)=PATM*PPP(I)                                             000241
00267             55 CONTINUE                                                                     000251
00271                CALL VARFMT(V,NPT)                                                           000251
00272                IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FAP,FB,(V(J),J=1,NPT)                       000255
00303                IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FPP,FB,(V(J),J=1,NPT)                       000301
00303          C   TEMPERATURE                                                      OUTP0047      000301
00314                FMT(3) = F13                                                                 000323
00315                FMT(4) = TWO                                                                 000325
00316                IF (IFLAG.EQ.0) GO TO 74                                                     000327
00320                DO 72 J=1,NPT                                                                000330
00323             72 TTT(J)=(TTT(J)-273.15)*1.8+32.                                               000334
00325             74 IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FTK,FB,(TTT(J),J=1,NPT)                     000342
00336                IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FTR,FB,(TTT(J),J=1,NPT)                     000365
00336          C   ENTHALPY                                                         OUTP0056      000365
00347                DO 75 I=1,NPT                                                  OUTP0058      000407
00352                V(I)=RBAR*HSUM(I)                                                            000420
00353                IF (IFLAG.EQ.1) V(I)=V(I)*1.8                                                000422
00355             75 CONTINUE                                                                     000431
00357                IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FH,FB,(V(J),J=1,NPT)                        000431
00370                IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FHH,FB,(V(J),J=1,NPT)                       000452
00370          C   ENTROPY                                                          OUTP0064      000452
00401                FMT(4) = FOUR                                                                000474
00402                DO 78 I = 1,NPT                                                              000501
00405             78 V(I) = RBAR*SSUM(I)                                                          000501
00407                IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FS,FB,(V(J),J=1,NPT)                        000504
00420                IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FSS,FB,(V(J),J=1,NPT)                       000525
00420          C     DENSITY                                                                      000525
00431                DO 70 I = 1,NPT                                                              000547
00436                IF (VLM(I).GT.0) V(I)=1./VLM(I)                                              000560
00436                IF (IFLAG.EQ.1) V(I)=V(I)*2206./35.31                                        000565
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00440    118*      70 CONTINUE                                                               000575
00442    119*         IF (IFLAG.EQ.0) WRITE (JOUT,1) (V(J),J=1,NPT)                          000575
00451    120*       1 FORMAT (1X,14HDENSITY G/CC  ,1P13E9.3)                                 000611
00452    121*         IF (IFLAG.EQ.1) WRITE (JOUT,2) (V(J),J=1,NPT)                          000611
00461    122*       2 FORMAT (1X,'DENSITY L/F**3',1P13E9.3)                                  000626
00462    123*         WRITE(JOUT,80)                                                         000626
00464    124*      80 FORMAT ( 1H )                                           OUTP0070       000633
00464    125*    C   MOLECULAR WEIGHT                                         OUTP0072       000633
00465    126*         WRITE(JOUT,FMT) FM,FB,(WM(J), J = 1,NPT)                               000633
00465    127*    C   (DLV/DLP)T                                               OUT            000633
00475    128*         IF (EQL)  WRITE(JOUT,FMT) F',FB,(DLVPT(J), J = 1,NPT)                  000652
00475    129*    C   (DLV/DLT)P                                               OUTP0083       000652
00506    130*         IF (EQL)  WRITE(JOUT,FMT) FV,FB,(DLVTP(J), J = 1,NPT)                  000673
00506    131*    C   HEAT CAPACITY                                            OUTP0087       000673
00517    132*         DO 85  I=1,NPT                                          OUTP0089       000717
00522    133*      85 V(I) = RBAR*CPR(I)                                                     000717
00524    134*         WRITE(JOUT,FMT) FCP,(V(J), J = 1,NPT)                                  000722
00524    135*    C   GAMMA(S)                                                 OUTP0093       000722
00533    136*         WRITE(JOUT,FMT) FG,FB,(GAMMAS(J), J = 1,NPT)                           000737
00533    137*    C   SONIC VELOCITY                                           OUTP0097       000737
00543    138*         FMT(4) = TWO                                                           000756
00544    139*         DO 95 I = 1,NPT                                         OUTP0100       000763
00547    140*      95 SONVEL(I) = SQRT(RBR*GAMMAS(I)*TTT(I)/WM(I))                           000763
00551    141*         WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(J), J = 1,NPT)                        000774
00561    142*         CALL MOVABS(500,50)                                                    001012
00562    143*         CALL HOLDIT                                                            001016
00563    144*         CALL PAGIT                                                             001020
00564    145*         RETURN                                                                 001022
00564    146*    C                                                        OUTP0104       001022
00565    147*         ENTRY OUT1                                                             001025
00566    148*         IF (CF+1.0) ,130,                                                      001025
00571    149*         COF=OF/CF                                                              001030
00572    150*         WRITE (JOUT,22) COF,WCR,PER                                            001033
00577    151*     130 WRITE (JOUT,80)                                                        001044
00601    152*         NO = 0                                                                 001050
00601    153*    C   MOLE FRACTIONS EQUILIBRIUM OR FROZEN                     OUT12270       001050
00602    154*         WRITE(JOUT,280)                                                        001051
00604    155*     280 FORMAT (15HOMOLE FRACTIONS/)                                           001056
00605    156*         IF (.NOT. EQL)  GO TO 175                                              001056
00605    157*    C   EQUILIBRIUM MOLE FRACTIONS                                              001056
00607    158*         DO 170 K=1,NS                                           OUT12330       001100
00612    159*         DO 140 I=1,NPT                                          OUT12340       001100
00615    160*     140 V(I) = EN(K,I)/TOTN(I)                                                 001100
00617    161*         DO 150 I=1,NPT                                          OUT12370       001106
00622    162*     150 IF (V(I) .GE. 5.0E-7)  GO TO 160                                       001106
00625    163*         NO = 1                                                                 001114
00626    164*         GO TO 170                                               OUT12400       001116
00627    165*     160 WRITE(JOUT,340) (SUB(K,J), J = 1,3),FB,(V(I), I = 1,NPT)               001120
00642    166*     340 FORMAT (1H ,3A4,A2,1P13E9.3)                                           001150
00643    167*     170 CONTINUE                                                OUT12430       001150
00643    168*    C   OUTPUT COMPLETE GO EXIT                                  OUT12590       001150
00645    169*         GO TO 211                                               OUT12600       001150
00645    170*    C   FROZEN MOLE FRACTIONS                                                   001150
00646    171*     175 J = 0                                                                  001152
00647    172*         DO 179 K = 1,NS                                         OUT12630       001152
00652    173*         V(J+1) = EN(K,1)/TOTN(1)                                               001164
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00653    174*          IF (V(J+1) .LT. 5.0E-7)  ND = 1                                         001170
00654    175*          IF (V(J+1) .LT. 5.0E-7)  GO TO 177                                      001177
00655    176*     C    OUTPUT VALUE ACCEPTED                                      OUT12660    001177
00657    177*          J = J + 1                                                               001204
00660    178*          DO 176 I = 1,3                                                          001207
00663    179*     176  Z(J,I) = SUB(K,I)                                                       001216
00665    180*     177  IF (J .NE. 4 .AND. K .NE. NS)  GO TO 179                                001221
00667    181*          IF (J .EQ. 0)  GO TO 180                                                001234
00671    182*          WRITE(JOUT,320) (Z(I,1),Z(I,2),Z(I,3),V(I), I = 1,J)                    001236
00702    183*     320  FORMAT (1H ,4(3A4,F11.8,5X))                                            001255
00703    184*          J = 0                                                                   001255
00704    185*     179  CONTINUE                                                   OUT12780    001264
00706    186*     180  IF (ND .EQ. 0)  GO TO 211                                               001261
00710    187*          WRITE(JOUT,290)                                                         001262
00712    188*     290  FORMAT (//1X,116HADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHO      001267
00712    189*         1SE MOLE FRACTIONS WERE LESS THAN 5.0E-7 FOR ALL ASSIGNED CONDITION      001267
00712    190*         2S//)                                                                    001267
00713    191*          J = 0                                                                   001267
00714    192*          DO 210 K=1,NS                                              OUT12780    001275
00717    193*          DO 190 I=1,NPT                                             OUT12790    001307
00722    194*     190  IF( (EN(K,I)/TOTN(I)) .GE. (5.0E-7) ) GO TO 200            OUT12800    001307
00725    195*          J = J + 1                                                               001317
00726    196*          DO 195 I = 1,3                                                          001322
00731    197*     195  Z(J,I) = SUB(K,I)                                                       001331
00733    198*     200  IF (J .NE. 10 .AND. K .NE. NS)  GO TO 210                               001334
00735    199*          IF (J .EQ. 0)  GO TO 211                                                001347
00737    200*          WRITE(JOUT,300) (Z(I,1),Z(I,2),Z(I,3), I = 1,J)                         001351
00747    201*     300  FORMAT (10(1X,3A4))                                        OUT13100    001367
00750    202*          J = 0                                                                   001367
00751    203*     210  CONTINUE                                                   OUT12900    001373
00751    204*     C    REMOVE TO IMPROVE PRINTOUT FOR COAL CALCULATIONS                        001373
00751    205*     C       WHICH ARE ALWAYS IN WEIGHT FRACTION                                  001373
00753    206*      211 RETURN                                                                  001373
00754  *DIAGNOSTIC*  CONTROL CAN NEVER REACH THE NEXT STATEMENT
00754    207*          IF (.NOT.MOLES) WRITE (JOUT,310)                                        001375
00757    208*     310  FORMAT (//1X,77HNOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND O      001404
00757    209*         1F OXIDANT IN TOTAL OXIDANTS)                                            001404
00760    210*          RETURN                                                                  001404
00761    211*          ENTRY OUT4                                                              001407
00762    212*          REAL LHVS,LHVD                                                          001407
00763    213*          DIMENSION CMW(13),XDP(13),YDPS(13),HHVS(13),EE(13),YDP(13),             001407
00763    214*         X   HHVD(13),LHVS(13),LHVD(13),DOL(13)                                   001407
00764    215*          DIMENSION ISUB(150,3)                                                   001407
00765    216*          EQUIVALENCE (ISUB(1,1),SUB(1,1))                                        001407
00766    217*          DIMENSION INDX(6)                                                       001407
00767    218*          DIMENSION IDG(6,3)                                                      001407
00770    219*          DATA (IDG(1,I),I=1,3)/'CO ',2*' '/                                      001407
00772    220*          DATA (IDG(2,I),I=1,3)/'CO2',2*' '/                                      001407
00774    221*          DATA (IDG(3,I),I=1,3)/'CH4',2*' '/                                      001407
00776    222*          DATA (IDG(4,I),I=1,3)/'H2 ',2*' '/                                      001407
01000    223*          DATA (IDG(5,I),I=1,3)/'N2 ',2*' '/                                      001407
01002    224*          DATA (IDG(6,I),I=1,3)/'AR',2*' '/                                       001407
01004    225*          WRITE (JOUT,490)                                                        001407
01006    226*      490 FORMAT (1H )                                                            001414
01007    227*          WRITE (JOUT,492) HHVV                                                   001414
01012    228*      492 FORMAT (1X,'HHV COAL B/LB',1X,F9.2)                                     001440
```

```
 01013    229*          DO 502 I=1,NPT                                                001440
 01016    230*          SUM=0.                                                        001440
 01017    231*          DO 500 J=1,NS                                                 001443
 01022    232*          IF (IUSE(J).NE.0) GO TO 500                                   001443
 01024    233*          SUM=SUM+EN(J,I)/TOTN(I)                                       001444
 01025    234*      500 CONTINUE                                                      001453
 01027    235*          CMW(I)=WM(I)*SUM                                              001453
 01030    236*      502 CONTINUE                                                      001461
 01032    237*          WRITE (JOUT,504) (CMW(I),I=1,NPT)                             001461
 01040    238*      504 FORMAT (1X,'MIXTURE MW',4X,13F9.3)                            001477
 01040    239*  C       LOCATE DRY ELEMENTS                                           001477
 01041    240*          DO 510 I=1,6                                                  001477
 01044    241*          DO 508 J=1,NS                                                 001510
 01047    242*          DO 506 K=1,3                                                  001520
 01052    243*          IF (IDG(I,K).NE.ISUB(J,K)) GO TO 508                          001520
 01054    244*      506 CONTINUE                                                      001527
 01056    245*          INDX(I)=J                                                     001527
 01057    246*          GO TO 510                                                     001531
 01060    247*      508 CONTINUE                                                      001534
 01062    248*          INDX(I)=0                                                     001534
 01063    249*      510 CONTINUE                                                      001540
 01065    250*          DO 516 I=1,NPT                                                001540
 01070    251*          SUM=0.                                                        001567
 01071    252*          DO 514 J=1,6                                                  001573
 01074    253*          IJ=INDX(J)                                                    001573
 01075    254*          IF (IJ.EQ.0) GO TO 514                                        001574
 01077    255*          SUM=SUM+EN(IJ,I)                                              001576
 01100    256*      514 CONTINUE                                                      001605
 01102    257*          XDP(I)=SUM/TOTN(I)                                            001605
 01103    258*      516 CONTINUE                                                      001612
 01105    259*          WRITE (JOUT,520) (XDP(I),I=1,NPT)                             001612
 01113    260*      520 FORMAT (1X,'MF OF CDG',5X,13F9.5)                             001627
 01114    261*          DO 522 I=1,NPT                                                001627
 01117    262*          YDPS(I)=(385.2*XDP(I)/CMW(I))*((1./CF)*(1.+OF))               001627
 01120    263*      522 CONTINUE                                                      001634
 01122    264*          WRITE (JOUT,524) (YDPS(I),I=1,NPT)                            001634
 01130    265*      524 FORMAT (1X,'Y SAT SCF/LB',2X,13F9.5)                          001646
 01131    266*          L1=INDX(1)                                                    001646
 01132    267*          L3=INDX(3)                                                    001650
 01133    268*          L4=INDX(4)                                                    001652
 01134    269*          DO 530 I=1,NPT                                                001662
 01137    270*          SUM=0.                                                        001675
 01140    271*          IF (L4.NE.0) SUM=SUM+319.24*EN(L4,I)/TOTN(I)                  001677
 01142    272*          IF (L1.NE.0) SUM=SUM+316.06*EN(L1,I)/TOTN(I)                  001710
 01144    273*          IF (L3.NE.0) SUM=SUM+994.4*EN(L3,I)/TOTN(I)                   001721
 01146    274*          HHVS(I)=SUM/XDP(I)                                            001732
 01147    275*      530 CONTINUE                                                      001737
 01151    276*          WRITE (JOUT,532) (HHVS(I),I=1,NPT)                            001737
 01157    277*      532 FORMAT (1X,'HHV SAT B/SCF',1X,13F9.2)                         001760
 01160    278*          DO 538 I=1,NPT                                                001760
 01163    279*          EE(I)=HHVS(I)*YDPS(I)/HHVV                                    001760
 01164    280*          YDP(I)=379.5*YDPS(I)/385.2                                    001764
 01165    281*          HHVD(I)=(385.2/379.5)*HHVS(I)                                 001770
 01166    282*          IF (L4.NE.0) LHVS(I)=HHVS(I)-(1059.9*18./385.2)*(EN(L4,I)/TOTN(I))  001773
 01166    283*         X   /XDP(I)                                                    001773
 01170    284*          LHVD(I)=LHVS(I)*385.2/379.5                                   002004
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     OUT1                                                                                DATE 101580        PAGE      8

  01171     285*          DOL(I)=10000.*(1.25*HHVV/10000.+OF/CF)/(HHVS(I)*YDPS(I))                002012
  01172     286*      538 CONTINUE                                                             002021
  01174     287*          WRITE (JOUT,542) (EE(I),I=1,NPT)                                     002021
  01202     288*      542 FORMAT (1X,'EFFICIENCY',4X,13F9.5)                                   002033
  01203     289*          WRITE (JOUT,544) (YDP(I),I=1,NPT)                                    002033
  01211     290*      544 FORMAT (1X,'Y DRY SCF/LB',2X,13F9.5)                                 002045
  01212     291*          WRITE (JOUT,546) (HHVD(I),I=1,NPT)                                   002045
  01220     292*      546 FORMAT (1X,'HHV DRY B/SCF',1X,13F9.2)                                002057
  01221     293*          WRITE (JOUT,548) (LHVS(I),I=1,NPT)                                   002057
  01227     294*      548 FORMAT (1X,'LHV SAT B/SCF',1X,13F9.2)                                002071
  01230     295*          WRITE (JOUT,550) (LHVD(I),I=1,NPT)                                   002071
  01236     296*      550 FORMAT (1X,'LHV DRY B/SCF',1X,13F9.2)                                002103
  01237     297*          WRITE (JOUT,552) (DOL(I),I=1,NPT)                                    002103
  01245     298*      552 FORMAT (1X,'$ PER MMBTU',3X,13F9.2)                                  002115
  01246     299*      560 CONTINUE                                                             002115
  01247     300*          RETURN                                                               002115
  01250     301*          END                                                       OUTP0137  002171

          END OF COMPILATION:           1 DIAGNOSTICS.

     @HDG,P       PROK
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      PROK                                                                                        DATE 101580        PAGE     1
@PDP,LWF   PROK,PROK
PDP12R1 R72-16 10/15/80 13:07:27 (0,0)        RI
PE0001         SPECPK PROC
  0002               COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)
  0003              1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)
  0004               DATA NSPP1/151/
  0005          END

END PDP  ERRORS : NONE


@HDG,P       REACT
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REACT                                                                                       DATE 101580        PAGE     1

@FOR,S    REACT,REACT
HSA  E3 -10/15/80-13:07:28 (31,)

   SUBROUTINE REACT       ENTRY POINT 001077

   STORAGE USED: CODE(1) 001111; DATA(0) 000367; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    HOLCON 000010
    0004    MISC    001701
    0005    INOX    000041
    0006    CCC     000003
    0007    CFUEL   000004

   EXTERNAL REFERENCES (BLOCK, NAME)

    0010     6OUT
    0011     NNCOD$
    0012     MOVAB$
    0013     HOLDIT
    0014     PAGIT
    0015     NREW$
    0016     NRBU$
    0017     NI02$
    0020     NI01$
    0021     NWDU$
    0022     NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    000327 101L       0001    000003 132G       0001    000013 143G       0001    000072 16L        0001    000074 20L
    0001    000463 200L       0001    000521 204L       0001    000106 206G       0001    000557 210L       0000    000315 212F
    0001    000566 214L       0001    000736 216L       0001    000740 220L       0001    001002 222L       0001    001005 224L
    0001    001022 226L       0001    001042 224L       0001    001056 230L       0001    000146 232G       0001    000233 267G
    0001    000243 275G       0000    000301 30F        0001    000256 304G       0001    000300 317G       0001    000377 342G
    0001    000226 37L        0001    000512 400G       0001    000534 414G       0001    000554 430G       0001    000617 447G
    0001    000270 45L        0001    000275 46L        0001    000662 460G       0001    000712 473G       0001    000311 50L
    0001    000766 510G       0001    000771 513G       0001    001012 531G       0001    001033 543G       0001    001046 552G
    0003    000042 6L         0004  R 000640 AM         0004    000705 AM1        0004  R 000707 ANAME      0004  R 001135 ANUM
    0004  R 000004 ATOM       0004    000514 BO         0004  R 000545 BOP        0005    000036 CALCH      0007  R 000000 CF
    0005    000001 CONVG      0004    000706 CPR1       0004    000634 CPSUM      0004  R 000654 DATA       0006    000002 DEMAND
    0004  R 001560 DENS       0003    000000 END        0004    001700 ENLSAV     0004    000000 ENN        0004    001676 ENNL
    0004    001677 ENSAVE     0004  R 001414 ENTH       0004    000636 EQRAT      0004  R 001445 FAZ        0004  I 001527 FOX
    0003    000001 GAS        0006    000000 GRAPH      0007  R 000001 HHVV       0005    000003 HP         0004  R 000642 HPP
    0004    000637 HSUBO      0000  I 000262 I          0005  I 000030 IC         0005    000000 IDEBUG     0003    000002 IE
    0005    000015 IMAT       0000    000344 INJPS      0000  I 000271 IO         0005    000023 IONS       0000  I 000235 IOUT
    0005    000021 IP         0005    000037 IQSAVE     0005    000016 IQ1        0005    000005 ISV        0005    000034 IT
    0003  I 000003 IZERO      0000  I 000266 J          0000  I 000275 JJ         0005    000026 JLIO       0006  I 000001 JOUT
    0005    000025 JSOL       0005    000031 JS1        0000  I 000265 K          0005    000014 KMAT       0005  I 000012 L
    0003  I 000004 LANK       0000  I 000145 LINE1      0000  I 000172 LINE2      0000  I 000215 LINE3      0004  I 000463 LLMT
    0000  I 000032 LLMTS      0005    000040 LSAVE      0003  I 000005 MOL        0000  I 000272 MOLE       0005  L 000006 MOLES
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      REACT                                                                                    DATE 101580        PAGE    2

      0000 I 000270 N          0004 I 000707 NAME       0000 I 000273 NAST       0005   000024 NC         0000 I 000300 NDUMMY
      0005 L 000022 NEWR       0000 I 000267 NFUEL      0005   000035 NFZ        0000 I 000000 NLS        0000 I 000277 NN1
      0005   000017 NOF        0005 I 000020 NOMIT      0005   000007 NP         0005   000011 NPT        0005 I 000027 NREAC
      0005   000013 NS         0005   000010 NT         0000 I 000263 N3         0000 I 000264 N8         0004   000635 OF
      0003 I 000006 OX         0004   001644 OXF        0000 R 000276 PCWT       0004 R 001363 PECWT      0007 R 000003 PER
      0004   000633 PP         0004 R 000644 RH         0004   001611 RHOP       0000 R 000274 RM         0004 R 001612 RMW
      0004 R 001476 RTEMP      0000 R 000063 SBOP       0005   000033 SHOCK      0005   000004 SP         0004   000001 SUMN
      0004   000003 SO         0004   000632 THIGH      0004   001643 TLN        0004   000630 TLOW       0004   000627 TM
      0004   000631 TMID       0005   000002 TP         0004   000002 TT         0000 R 000001 V          0004 R 000646 VMIN
      0005   000032 VOL        0004 R 000650 VPLS       0007 R 000002 WCR        0004 R 000652 WP         0003 I 000007 ZERO


 00101      1*          SUBROUTINE REACT                                                                   000003
 00101      2*    C                                                                                        000003
 00103      3*          COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                      /HOLCON/    000003
 00104      4*          COMMON /MISC/ EMN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                          000003
 00104      5*         1               BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                     000003
 00104      6*         2               HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),         /MISC/      000003
 00104      7*         3               DATA(25),AM1,CPR1,NAME(25,6),AMUM(25,6),PECWT(25),                  000003
 00104      8*         4               ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,                   000003
 00104      9*         5               RMW(25),TLN,OXF(26),ENML,ENSAVE,ENLSAV                              000003
 00105     10*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,WP,NT,NPT,L,NS,          /INDX/      000003
 00105     11*         1               KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,      /INDX/      000003
 00105     12*         2               NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE        /INDX/      000003
 00105     13*    C                                                                                        000003
 00106     14*            COMMON /CCC/ GRAPH,JOUT,DEMAND                                                   000003
 00106     15*    C                                                                                        000003
 00107     16*          COMMON /CFUEL/CF,HHVV,WCR,PER                                                      000003
 00110     17*          DATA NLS/0/                                                                        000003
 00112     18*          DIMENSION ANAME(25,6),V(25),LLMTS(25),SBOP(25,2)                                   000003
 00113     19*          EQUIVALENCE (NAME,ANAME)                                                           000003
 00114     20*          INTEGER FOX,OX,ZERO                                                                000003
 00115     21*          LOGICAL MOLES,NEWR                                                                 000003
 00116     22*          DIMENSION LINE1(21),LINE2(19),LINE3(16)                                            000003
 00117     23*          DIMENSION IOUT(21)                                                                 000003
 00120     24*          DATA (LINE1(I),I=1,21)/' INDEX',4*'      ',                                      000003
 00120     25*         X   'REACTA','NT(*) ',3*'      ','      R',                                        000003
 00120     26*         X   'EL WT/','   MOL','E  ENT','HALPY/',                                          000003
 00120     27*         X   '   PHA','SE  TE','MP,K  ',' FUEL/','  DENS','ITY   '/                        000003
 00122     28*          DATA (LINE2(I),I=1,19)/10*'      ',                                             000003
 00122     29*         X   '     N','O MOLE','S     ','  INT',                                           000003
 00122     30*         X   ' ENERG','Y     ',2*'      ',' OXID '/                                        000003
 00124     31*          DATA (LINE3(I),I=1,16)/8*'      ',                                              000003
 00124     32*         X   '  *   ','   IND','ICATES',' ENTHA','LPY TO',' BE CA',                         000003
 00124     33*         X   'LCULAT','ED    '/                                                            000003
 00124     34*    C                                                                                        000003
 00126     35*          DATA N3/8/,N8/12/                                                                  000003
 00131     36*                                                                                             000003
 00131     37*    C                                                                          RCTN0022      000003
 00131     38*          DO 8 K = 1,2                                                                       000003
 00134     39*          WP(K)=0.                                                                           000003
 00135     40*          HPP(K)=0.                                                                          000003
 00136     41*          RH(K)=0.                                                                           000004
 00137     42*          VPLS(K)=0.                                                                         000005
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00140    43.          VMIN(K)=0.                                                  000006
00141    44.          AM(K)=0.                                                    000007
00142    45.          DO 8 J=1,25                                                 000013
00145    46.          LLMT(J)=0                                                   000013
00146    47.      8   BOP(J,K) = 0.0                                              000013
00151    48.          NFUEL = 0                                                   000017
00152    49.          N=1                                                         000020
00152    50.    C     WRITE REACTANT HEADER                                       000020
00153    51.          CALL GOUT(LINE1,126)                                        000022
00154    52.          CALL GOUT(LINE2,114)                                        000026
00155    53.          L=1                                                         000032
00156    54.          IO=43                                                       000034
00156    55.    C     READ REACTANTS                                              000034
00157    56.             REWIND IO                                                000036
00160    57.        6 READ (IO) NREAC,CF                                          000042
00164    58.       10 IF (IO.EQ.NB) GO TO 20                                      000047
00166    59.          IF (CF,1.0) ,18,                                            000052
00171    60.          REWIND IC                                                   000066
00172    61.          READ (NB) NREAC,CF,HH,VV,CR,PER                             000060
00201    62.       18 IF (NREAC.EQ.0.0) GO TO 200                                 000072
00203    63.    20       CONTINUE                                                 000074
00204    64.          READ (IO) (NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),  000074
00204    65.         X   NAME(N,6),ANUM(N,6),FAZ(N),                              000074
00204    66.         X   RTEMP(N),FOX(N),DENS(N)                                  000074
00224    67.          NAST=1H                                                     000124
00225    68.          IF (NAME(N,6).EQ.2HOO) NAST=1H*                             000127
00227    69.          ENCODE (30,IOUT) N,(NAME(N,J),ANUM(N,J),J=1,5),PECWT(N),MOLE,  000135
00227    70.         X   ENTH(N),NAST,FAZ(N),RTEMP(N),FOX(N),DENS(N)              000135
00247    71.          CALL GOUT(IOUT,126)                                         000164
00250    72.       30 FORMAT (1X,I2,2X,5(A2,F8.4,2X),F10.6,2X,A1,F13.4,A1,3X,A1,F12.3,  000170
00250    73.         X   3X,A1,F12.5,1X)                                          000170
00251    74.          IF(L.EQ.0)GO TO 20                                          000170
00253    75.          IF (MOLE .EQ. MOL)  MOLES = .TRUE.                          000172
00253    76.    C     IF OXIDANT, K = 1; IF FUEL, K = 2.                          000172
00255    77.          IF(FOX(N).EQ.ZERO)  FOX(N)=OX                               000177
00257    78.          IF (PECWT(N) .LE. 0.0)  PECWT(N) = 1.0                      000205
00261    79.          K = 1                                                       000213
00262    80.          IF(FOX(N).EQ.OX)  GO TO 37                                  000215
00264    81.          K = 2                                                       000221
00265    82.          NFUEL = NFUEL+1                                             000223
00266    83.       37 DO 38 J=1,25                                                000226
00271    84.       38 DATA(J) = 0.0                                               000233
00273    85.          RM=0.                                                       000234
00274    86.          DO 100 JJ=1,6                                               000243
00277    87.          IF (ANUM(N,JJ) .LE. 0.0)  GO TO 101                         000243
00301    88.          IF (NAME(N,JJ) .EQ. ZERO)  NAME(N,JJ) = OX                  000246
00303    89.          DO 41 J=1,15                                                000256
00306    90.          I = J                                                       000256
00307    91.          IF(LLMT(J).EQ.0) GO TO 45                                   000260
00311    92.      41  IF (NAME(N,JJ) .EQ. LLMT(J))  GO TO 46                      000262
00314    93.      45  L = I                                                       000270
00315    94.          LLMT(J)=NAME(N,JJ)                                          000272
00316    95.      46  DO 48 I = 1,101                                             000300
00321    96.      48  IF (ATOM(1,I) .EQ. ANAME(N,JJ))  GO TO 50                   000300
00324    97.          L=0                                                         000306
00325    98.          GO TO 20                                                    000307
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ORIGINAL PAGE IS
OF POOR QUALITY

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00326      99*      50  RM = RM + ANUM(N,JJ)*ATOM(2,I)                                 000311
00327     100*          V(J) = ATOM(J,I)                                               000317
00330     101*     100  DATA(J) = ANUM(N,JJ)                                           000321
00332     102*     101 PCWT=PECWT(N)                                                   000327
00333     103*          IF(MOLES) PCWT=PCWT*RM                                         000332
00335     104*          WP(K)=WP(K) + PCWT                                             000337
00336     105*          IF (NAME(N,6).NE.IZERO) HPP(K)=HPP(K)+ENTH(N)*PCWT/RM          000343
00340     106*          AM(K)=AM(K)+PCWT/RM                                            000365
00341     107*          DO 110  J=1,L                                                  000377
00344     108*     110  BOP(J,K) = DATA(J)*PCWT/RM + BOP(J,K)                          000377
00346     109*          IF (DENS(N) .GT. 0.0)  RH(K) = RH(K) + PCWT/DENS(N)            000404
00350     110*          RMW(N) = RM                                                    000416
00351     111*          N = N+1                                                        000420
00352     112*          IF (N.EQ.26) GO TO 200                                         000423
00354     113*          IF (IO.EQ.N3.AND.N-1.EQ.NREAC) GO TO 200                       000425
00356     114*          IF (IO.EQ.N8.AND.N-1.EQ.NN1+NREAC) GO TO 200                   000442
00360     115*          GO TO 20                                                       000461
00361     116*     200 NN1=N-1                                                         000463
00362     117*          IF (IO.EQ.N8) GO TO 204                                        000465
00364     118*          IO=N8                                                          000470
00365     119*          REWIND IO                                                      000472
00366     120*          READ (IO) NREAC,CF,HHVV,WCR,PER                                000475
00375     121*          IF (NREAC.EQ.0) GO TO 204                                      000506
00377     122*          DO 202 I=1,4                                                   000513
00402     123*          READ (IO) NDUMMY                                               000512
00405     124*     202 CONTINUE                                                        000517
00407     125*          GO TO 6                                                        000517
00410     126*     204 NREAC=NN1                                                       000521
00411     127*          IF(NFUEL.GT.0)  GO TO 210                                      000522
00411     128*    C     100 PERCENT OXIDANT, CALL REACTANTS FUEL                       000522
00413     129*          DO 205  N=1,NREAC                                              000534
00416     130*     205  FOX(N) = LANK                                                  000534
00420     131*          RH(2) = RH(1)                                                  000536
00421     132*          RH(1) = 0.                                                     000540
00422     133*          WP(2) = WP(1)                                                  000541
00423     134*          WP(1) = 0.                                                     000543
00424     135*          HPP(2) = HPP(1)                                                000544
00425     136*          AM(2) = AM(1)                                                  000546
00426     137*          AM(1) = 0.                                                     000550
00427     138*          DO 208  J=1,L                                                  000554
00432     139*     208  BOP(J,2) = BOP(J,1)                                            000554
00434     140*     210 IF (L.NE.0) GO TO 214                                           000557
00436     141*          WRITE (JOUT,212)                                               000560
00440     142*     212 FORMAT ('0','ERROR IN REACTANT DATA')                           000566
00441     143*     214 CALL GOUT(' ',1)                                                000566
00442     144*          CALL GOUT(LINE3,96)                                            000571
00443     145*          CALL MOVABS(500,50)                                            000575
00444     146*          CALL HOLDIT                                                    000601
00445     147*          CALL PAGIT                                                     000603
00446     148*          DO 220 K=1,2                                                   000605
00451     149*          IF (WP(K) .LE. 0.0)  GO TO 220                                 000637
00453     150*          HPP(K)=HPP(K)/WP(K)                                            000642
00454     151*          AM(K) = WP(K)/AM(K)                                            000645
00455     152*          IF (RH(K) .GT. 0.0)  RH(K) = WP(K)/RH(K)                       000650
00457     153*          DO 215 J=1,L                                                   000662
00462     154*          BOP(J,K)=BOP(J,K)/WP(K)                                        000662
```

```
 00463    155.          IF(V(J).LT.0.)VMIN(K)= VMIN(K)+BOP(J,K)*V(J)                        000664
 00465    156.     215  IF (V(J) .GT. 0.0)  VPLS(K) = VPLS(K) + BOP(J,K)*V(J)               000673
 00470    157.          IF(MOLES) GO TO 220                                                 000705
 00472    158.          DO 218 N=1,NREAC                                                    000712
 00475    159.          IF((FOX(N).EQ.OX.AND.K.EQ.2).OR.(FOX(N).NE.OX.AND.K.EQ.1))GOTO218   000712
 00477    160.          PECNT(N) = PECNT(N)/WP(K)                                           000732
 00500    161.     218  CONTINUE                                                            000742
 00502    162.     220  CONTINUE                                                            000742
 00504    163.          NEWR=.TRUE.                                                         000742
 00504    164.   C  ARE ELEMENTS SAME AS FOR  LAST SET OF REACTANTS, IF SO, NEWR=.FALSE.  4/23/70  000742
 00505    165.          IF (L .NE. NLS .OR. NOMIT .NE. 0)  GO TO 226                        000744
 00507    166.          DO 224 I=1,NLS                                                      000756
 00512    167.          DO 222 J = 1,L                                                      000771
 00515    168.          IF(LLMT(J).NE.LLMTS(I))  GO TO 222                                  000771
 00517    169.          SBOP(I,1) = BOP(J,1)                                                000774
 00520    170.          SBOP(I,2) = BOP(J,2)                                                000776
 00521    171.          GO TO 224                                                           001000
 00522    172.     222  CONTINUE                                                            001003
 00524    173.          GO TO 226                                                           001003
 00525    174.     224  CONTINUE                                                            001006
 00527    175.          NEWR = .FALSE.                                                      001006
 00530    176.          DO 225 I = 1,L                                                      001012
 00533    177.          LLMT(I) = LLMTS(I)                                                  001012
 00534    178.          BOP(I,1)  = SBOP(I,1)                                               001013
 00535    179.     225  BOP(I,2) = SBOP(I,2)                                                001015
 00537    180.          GO TO 229                                                           001020
 00540    181.     226  NLS = L                                                             001022
 00541    182.          REWIND 4                                                            001023
 00542    183.          DO 228 I = 1,L                                                      001026
 00545    184.          SBOP(I,1) = BOP(I,1)                                                001033
 00546    185.          SBOP(I,2) = BOP(I,2)                                                001034
 00547    186.     228  LLMTS(I) = LLMT(I)                                                  001036
 00551    187.     229  DO 230  N=1,NREAC                                                   001042
 00554    188.          IF (DENS(N) .GT. 0.0)  GO TO 230                                    001046
 00556    189.          RH(2) = 0.                                                          001050
 00557    190.          RH (1) = 0.                                                         001051
 00560    191.          RETURN                                                              001052
 00561    192.     230  CONTINUE                                                            001057
 00563    193.          RETURN                                                              001057
 00564    194.          END                                                      RCTM0111   001110

       END OF COMPILATION:        NO  DIAGNOSTICS.


 @HDG,P      RKTOUT
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```
@FOR,S    RKTOUT,RKTOUT
MSA  E3 -10/15/80-13:07:33 (12,)

    SUBROUTINE RKTOUT     ENTRY POINT 000532

    STORAGE USED: CODE(1) 000541; DATA(0) 000122; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003    CONSTS 000006
     0004    POINTS 000335
     0005    SPECES 017106
     0006    INDX   000041
     0007    PERF   000166
     0010    OUPT   000073
     0011    CCC    000003
     0012    CFUEL  000001

    EXTERNAL REFERENCES (BLOCK, NAME)

     0013    MOVABS
     0014    OUT1
     0015    VARFMT
     0016    OUT2
     0017    GAMEFF
     0020    OUT3
     0021    OUT4
     0022    NWDU$
     0023    NI02$
     0024    NI01$
     0025    SQRT
     0026    NI03$
     0027    NERR3$

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001     000063 1466     0000     000066 150F     0001     000074 1546     0001     000121 1706     0001     000150 2006
     0001     000202 200L     0000     000075 208F     0001     000422 220L     0001     000235 2226     0001     000263 2366
     0001     000316 2546     0001     000340 2666     0001     000350 2746     0001     000366 3056     0001     000511 312L
     0001     000416 3216     0001     000427 3266     0001     000445 3376     0001     000466 3506     0001     000505 3606
     0000     000006 37F      0000     000027 38F      0000     000056 40F      0001     000520 400L     0000     000047 737F
     0005     011052 A        0007 R 000150 AEAT      0007 R 000133 APP       0003 R 000000 ATMN      0000 R 000002 AW
     0006     000036 CALCH    0012 R 000000 CF        0005     000000 COEF     0006     000001 CONVG    0004     000032 CPR
     0000 R 000005 CSTR       0005     010624 DELN     0011     000002 DEMAND   0004     000064 DLVPT    0004     000047 DLVTP
     0005     004312 EN       0005     010150 ENLN     0007 L 000165 EOL       0010 R 000002 FA        0010     000003 FAP
     0010 R 000005 FB         0010 R 000006 FC        0010     000007 FCP      0010 R 000012 FCST      0010 R 000014 FCV
     0010 R 000015 FG         0010 R 000017 FGE       0010 R 000020 FGV       0010     000021 FH       0010 R 000023 FI
     0010 R 000025 FIV        0010     000027 FM      0010 R 000031 FMT       0010 R 000050 FN        0010 R 000052 FOUR
     0010 R 000053 FP         0010     000054 FS      0010     000056 FSV      0010     000057 FT       0010     000061 FTK
     0010     000063 FV       0010 R 000065 FVEL      0010 R 000001 F13       0010 R 000000 F9X       0004 R 000101 GAMMAS
     0003 R 000001 GMET       0011     000000 GRAPH    0006     000003 HP       0004 R 000000 HSUM      0005 R 010376 HO
     0000 I 000004 I          0006     000030 IC      0006     000000 IDEBUG   0006     000015 IMAT     0000     000105 INJP$
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0006     000023 IONS       0006     000021 IP         0006     000037 IOSAVE     0006     000016 IQ1        0006     000005 ISV
0006   I 000034 IT         0005     016266 IUSE       0006     000026 JLIQ       0011   I 000001 JOUT       0006     000025 JSOL
0006     000031 JS1        0000   I 000003 K          0006     000014 KMAT       0006     000040 LSAVE      0006     000006 MOLES
0006     000024 NC         0006     000022 NEWR       0006     000035 NFZ        0006     000012 NLM        0006     000017 NOF
0006     000020 NOMIT      0006     000007 NP         0006   I 000011 NPT        0006     000027 NREAC      0006     000013 NS
0000   I 000000 NSPP1      0006     000010 NT         0010   I 000067 ONE        0004     000116 P          0003   R 000002 PATM
0007     000000 PCP        0004   R 000217 PPP        0003     000003 RBAR       0003   R 000004 RBR        0003     000005 RVR
0005     004060 S          0006     000033 SHOCK      0005     016660 SLN        0004   R 000251 SONVEL     0006     000004 SP
0007   R 000047 SPIM       0004     000015 SSUM       0005     015364 SUB        0007     000101 SUBAR      0007     000116 SUPAR
0004   R 000150 T          0000   R 000001 TEM        0005     016514 TEMP       0010   R 000070 THREE      0004     000320 TOTN
0006     000002 TP         0004   R 000266 TTT        0010   R 000071 TWO        0004   R 000202 V          0007   R 000064 VACI
0004     000303 VLM        0007   R 000032 VMOC       0006     000032 VOL        0004   R 000234 WM         0010     000072 ZERO


00101      1*           SUBROUTINE RKTOUT (IGAM)                                                   000000
00101      2*      C                                                                               000000
00101      3*      C  ROCKET PERFORMANCE PARAMETERS                                                000000
00101      4*      C                                                                  ROUT0001     000000
00103      5*           COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                   /CONSTS/     000000
00104      6*           COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                000000
00104      7*          1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)           000000
00104      8*          2 ,VLM(13),TOTN(13)                                                         000000
00104      9*      C    COMMON/SPECES,COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)            000000
00104     10*      C   1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)             000000
00105     11*           INCLUDE SPECPK                                                             000000
00111     12*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,  /INDX/    000000
00111     13*          1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/    000000
00111     14*          2              NREAC,IC,JS1,VOL,SHOCK,II,NFZ,CA,CM,IOSAVE,I,AXE    /INDX/    000000
00112     15*           COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),       /PERF/    000000
00112     16*          1              SUPAR(13),APP(13),AEAT(13),EQL                      /PERF/    000000
00113     17*           COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),   /OUPT/    000000
00113     18*          1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(18),FN(2),FOUR, /OUPT/   000000
00113     19*          2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,  /OUPT/    000000
00113     20*          3              TWO,ZERO                                            /OUPT/    000000
00113     21*      C                                                                               000000
00114     22*           COMMON /CCC/ GRAPH,JOUT,DEMAND                                             000000
00114     23*      C                                                                               000000
00115     24*           COMMON /CFUEL/CF                                                           000000
00116     25*           LOGICAL EQL                                                                000000
00117     26*           CALL MOVABS(500,50)                                                        000000
00120     27*           IF(EQL) WRITE(JOUT,37)                                                     000003
00123     28*        37 FORMAT(1H1/24X,84HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRROCK0090 000012
00123     29*          1IUM COMPOSITION DURING EXPANSION          ///)                             000012
00124     30*           IF (.NOT.EQL) WRITE(JOUT,38)                                               000012
00127     31*        38 FORMAT(1H1,26X,78HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN CROCK0107  000023
00127     32*          1OMPOSITION DURING EXPANSION          ///)                        ROCK0108  000023
00130     33*           IF(TTT(1).EQ.T(IT)) WRITE(JOUT,737)                                        000023
00133     34*       737 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE      )                           000034
00134     35*           TEM = PATM*PPP(1)                                                          000034
00135     36*           AW = ATMN*PPP(1)                                                           000037
00136     37*           WRITE(JOUT,40) TEM,AW                                                      000042
00142     38*        40 FORMAT (5H PC =,F10.3,7H PSIA =,1PE13.6,7H N/M**2)                         000051
00143     39*           CALL OUT1                                                                  000051
00144     40*           K = NPT - 2                                                                000053
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00145     41*           DO 20 I = 1,K                                                         000056
00150     42*       20  V(I) = 4HEXIT                                                         000063
00152     43*           WRITE(JOUT,150) (V(I), I = 1,K)                                       000065
00160     44*      150  FORMAT (1H0,16X,16HCHAMBER   THROAT,11(5X,A4))           RKT01590    000077
00160     45*      C    PRESSURE RATIOS                                           OUTP0030    000077
00161     46*           FMT(3) = ONE                                                          000077
00162     47*           CALL VARFMT (APP,NPT)                                                 000101
00163     48*           WRITE(JOUT,FMT) FP,FB,FB,(APP(I), I = 1,NPT)                          000105
00174     49*           CALL OUT2                                                             000124
00175     50*           IF (NPT .LT. 2)  GO TO 312                                            000126
00177     51*           DO 202 K=2,NPT                                            ROUT0028    000136
00202     52*           SPIM(K) = SQRT(2.0*RBR*(HSUM(1) - HSUM(K)))/GMET                      000150
00202     53*      C  AW (A/W) IN UNITS OF SEC/ATM                                            000150
00203     54*           AW = RBR*TTT(K)/(PPP(K)*WM(K)*SPIM(K)*GMET**2)                        000161
00204     55*           IF(K.NE.2)GO TO 200                                       ROUT0031    000171
00206     56*           CSTR = GMET*AW*PPP(1)                                                 000174
00207     57*           AEAT(2) = 1.                                                          000177
00210     58*      200  VACI(K)=SPIM(K)+PPP(K)*AW                                             000202
00211     59*           IF (SONVEL(K) .GT. 0.0)  VMOC(K) = GMET*SPIM(K)/SONVEL(K)             000205
00213     60*      202  V(K) = GMET*SPIM(K)                                                   000214
00215     61*           V(1) = 0.0                                                            000221
00216     62*           WRITE(JOUT,FMT) FGV,FVEL,(V(I), I = 1,NPT)                            000222
00216     63*      C    MACH NUMBER                                               ROUT0040    000222
00226     64*           FMT(4) = FOUR                                                         000240
00227     65*           VMOC(1)=0.                                                ROUT0042    000242
00230     66*           IF (GAMMAS(2) .LE. 0.0)  VMOC(2) = 0.0                                000243
00232     67*           WRITE(JOUT,FMT) FN,FB,(VMOC(I), I = 1,NPT)                            000247
00242     68*           WRITE(JOUT,208)                                                       000266
00244     69*      208  FORMAT (1H )                                              ROUT0048    000273
00244     70*      C    AREA RATIO                                                ROUT0062    000273
00245     71*           CALL VARFMT (AEAT,NPT)                                                000273
00246     72*           FMT(3) = F9X                                                          000301
00247     73*           WRITE(JOUT,FMT) FA,FB,FB,(AEAT(I), I = 2,NPT)                         000303
00247     74*      C    CSTAR                                                                 000303
00260     75*           FMT(4) = F13                                                          000321
00261     76*           FMT(5) = TWO                                                          000323
00262     77*           WRITE(JOUT,FMT) FCST,FB,(CSTR, I = 2,NPT)                             000325
00262     78*      C    CF - THRUST COEFICIENT                                    ROUT0055    000325
00272     79*           FMT(5) = FOUR                                                         000343
00273     80*           DO 212  I=2,NPT                                           ROUT0057    000350
00276     81*      212  V(I) = GMET*SPIM(I)/CSTR                                              000350
00300     82*           WRITE(JOUT,FMT) FC,FB,FB,(V(I), I = 2,NPT)                            000354
00311     83*           IF (IGAM .EQ. 0)  GO TO 220                                           000371
00311     84*      C    EFFECTIVE GAMMA                                                       000371
00313     85*           CALL GAMEFF (V,GAMMAS,APP,NPT,MO)                                     000373
00314     86*           WRITE(JOUT,FMT) FG(1),FGE,FB,(MO(I), I = 2,NPT)                       000402
00314     87*      C    VACUUM THRUST COEFFICIENT                                 RKT01050    000402
00325     88*      220  DO 230 I = 2,NPT                                                      000422
00330     89*      230  V(I) = GMET*VACI(I)/CSTR                                              000427
00332     90*           WRITE(JOUT,FMT) FCV,FB,FB,(V(I), I = 2,NPT)                           000433
00332     91*      C    VACUUM IMPULSE                                            ROUT0067    000433
00343     92*           FMT(5) = THREE                                                        000450
00344     93*           WRITE(JOUT,FMT) FIV,FB,(VACI(I), I = 2,NPT)                           000452
00344     94*      C    SPECIFIC IMPULSE                                          ROUT0071    000452
00354     95*           WRITE(JOUT,FMT) FI,FB,(SPIM(I), I = 2,NPT)                            000471
00354     96*      C    FROZEN MOLE FRACTION OUTPUT MOVED TO SUBROUTINE OUT3      RKT01400    000471
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00364     97*      312 CALL OUT3                                            000511
00365     98*          IF (CF*1.0) ,400,                                    000512
00370     99*          CALL OUT4                                            000515
00371    100*      400 CONTINUE                                             000520
00372    101*          RETURN                                               000520
00373    102*          END                                                  000540

       END OF COMPILATION:        NO  DIAGNOSTICS.

 aHDG.P     ROCKET
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@FOR,S    ROCKET,ROCKET
HSA  E3 -10/15/80-13:07:36 (10,)

    SUBROUTINE ROCKET     ENTRY POINT 001310

    STORAGE USED: CODE(1) 001317; DATA(0) 000231; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003    CONSTS  000006
     0004    POINTS  000335
     0005    MISC    001701
     0006    INDX    000041
     0007    PERF    000166
     0010    CCC     000003

    EXTERNAL REFERENCES (BLOCK, NAME)

     0011    NEWOF
     0012    FROZEN
     0013    EQLBRM
     0014    RKTOUT
     0015    SAVE
     0016    NWDU$
     0017    NIO2$
     0020    NRNL$
     0021    NWNL$
     0022    XPRR
     0023    ALOG
     0024    EXP
     0025    XPDR
     0026    SQRT
     0027    NERR3$

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001    000013 1256     0001    000162 1332L    0001    000035 1446     0001    000054 156G     0000    000104 1811F
     0001    000302 191L     0001    000420 192L     0000    000101 194F     0001    000261 195L     0001    000126 2036
     0000    000065 302F     0001    000026 303L     0001    000045 306L     0001    000103 321L     0001    000122 322L
     0001    000153 331L     0001    000160 332L     0001    000175 333L     0001    000213 334L     0001    000610 799L
     0001    000536 800L     0001    000763 802L     0001    000640 805L     0001    000703 809L     0001    000653 810L
     0001    001007 820L     0000    000125 821F     0001    001015 830L     0001    001043 834L     0001    001053 835L
     0001    001055 859L     0001    001061 860L     0000    000137 862F     0000    000166 865F     0001    001121 870L
     0001    001135 880L     0001    000457 899L     0001    000477 900L     0000    000073 923F     0001    000416 925L
     0001    001171 990L     0001    001232 997L     0001    001264 999L     0007 R  000150 AEAT     0000 R  000037 AEATL
     0005    000640 AM       0005    000705 AM1      0005    001135 ANUM     0007 R  000133 APP      0000 R  000035 APPL
     0000 R  000033 ARATIO   0000 L  000005 AREA     0000 D  000001 ASQ      0003    000000 ATMN     0005    000004 ATOM
     0000 R  000030 AWT      0005    000514 BO       0005    000545 BOP      0006    000036 CALCH    0006    000001 CONV6
     0004 R  000032 CPR      0000 R  000023 CPRF     0005    000706 CPR1     0005 R  000634 CPSUM    0005    000654 DATA
     0010    000002 DEMAND   0005    001560 DENS     0000 R  000026 DH       0000 R  000032 DLNP     0000 R  000040 DLNPE
     0000 R  000027 DLT      0004    000064 DLVPT    0004 R  000047 DLVTF    0000 R  000034 ELN      0005    001700 ENLSAV
     0005 R  000000 ENN      0005    001676 ENNL     0005    001677 ENSAVE   0005    001414 ENTH     0007 L  000165 EQL
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   0005      000636 EQRAT      0005      001445 FAZ        0005      001527 FOX        0000 L 000006 FROZ       0004 R 000101 GAMMAS
   0003      000001 GMET       0010      000000 GRAPH      0006 L 000003 HP         0005      000642 HPP        0005      000637 HSUBO
   0004 R 000000 HSUM       0000 I 000012 I          0006      000030 IC         0000 I 000000 ICASE      0006 I 000000 IDEBUG
   0000 I 000011 IGAM       0006      000015 IMAT       0000      000215 INJPS      0000 I 000016 IOF        0006      000023 IONS
   0006 I 000021 IP         0000 I 000022 IPP        0006      000037 IQSAVE     0006      000016 IQ1        0000 I 000020 ISUB
   0000 I 000021 ISUP       0006 I 000005 ISV        0006 I 000034 IT         0000 I 000017 ITNUM      0000 I 000025 ITROT
   0006      000026 JLIQ       0010 I 000001 JOUT       0006 I 000025 JSOL       0006      000031 JS1        0006      000014 KMAT
   0005      000463 LLMT       0006      000040 LSAVE      0006      000006 MOLES      0005      000707 NAME       0006      000024 NC
   0006      000022 NEWR       0006 I 000035 NFZ        0006      000012 NLM        0006 I 000017 NOF        0006      000020 NOMIT
   0006 I 000007 NP         0000 I 000013 NPP        0006 I 000011 NPT        0006      000027 NREAC      0006      000013 NS
   0000 I 000014 NSUB       0000 I 000015 NSUP       0006 I 000010 NT         0005 R 000635 OF         0005 R 001644 OXF
   0004 R 000116 P          0003      000002 PATM       0007 R 000000 PCP        0000 R 000031 PCPLT      0005      001363 PECWT
   0005 R 000633 PP         0004 R 000217 PPP        0003      000003 RBAR       0003 R 000004 RBR        0005      000644 RH
   0005      001611 RHOP       0000      000041 RKTINP     0005      001612 RMW        0005      001476 RTEMP      0003      000005 RVR
   0000 L 000007 SEQL       0006      000033 SHOCK      0004      000251 SONVEL     0006 L 000004 SP         0007      000047 SPIM
   0004 R 000015 SSUM       0007 R 000101 SUBAR      0005      000001 SUMN       0007 R 000116 SUPAR      0005 R 000003 SO
   0004 R 000150 T          0000 L 000010 THI        0005      000632 THIGH      0005      001643 TLN        0005      000630 TLOW
   0005      000627 TM         0000 R 000024 TMELT      0005      000631 TMID       0000 R 000036 TOL        0004      000320 TOTN
   0006 L 000002 TP         0005 R 000002 TT         0004 R 000266 TTT        0000 D 000003 USQ        0004      000202 V
   0007      000064 VACI       0004      000303 VLM        0005      000646 VMIN       0007      000032 VMOC       0006      000032 VOL
   0005      000650 VPLS       0004 R 000234 WM         0005      000652 WP


00101        1*          SUBROUTINE ROCKET                                                      ROCK0002      000000
00101        2*     C                                                                           ROCK0001      000000
00101        3*     C    ROCKET PERFORMANCE                                                     ROCK0004      000000
00101        4*     C                                                                                         000000
00103        5*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                           /CONSTS/      000000
00104        6*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                          000000
00104        7*          1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                     000000
00104        8*          2 ,VLM(13),TOTN(13)                                                                  000000
00105        9*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                            000000
00105       10*          1               BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                      000000
00105       11*          2               HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),       /MISC/        000000
00105       12*          3               DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),                   000000
00105       13*          4               ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,                    000000
00105       14*          5               RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                               000000
00106       15*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,       /INDX/        000000
00106       16*          1               KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,    /INDX/        000000
00106       17*          2               NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE      /INDX/        000000
00107       18*          COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),           /PERF/        000000
00107       19*          1               SUPAR(13),APP(13),AEAT(13),EQL                        /PERF/        000000
00107       20*     C                                                                                         000000
00110       21*            COMMON /CCC/ GRAPH,JOUT,DEMAND                                                     000000
00110       22*     C                                                                                         000000
00111       23*          DATA ICASE/0/                                                                        000000
00113       24*          DOUBLE PRECISION ASQ,USQ                                                             000000
00114       25*          LOGICAL AREA,EQL,FROZ,HP,SEQL,SP,THI,TP                                              000000
00114       26*     C                                                                                         000000
00115       27*          NAMELIST /RKTINP/ EQL,FROZ,IGAM,PCP,SUBAR,SUPAR                       /RKTINP/      000000
00115       28*     C                                                                                         000000
00116       29*          NFZ = 1                                                                              000000
00117       30*          APP(1) = 1.                                                                          000001
00120       31*          IF (ICASE .GT. 0)  GO TO 303                                                         000003
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ORIGINAL PAGE IS
OF POOR QUALITY

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 00122    32*               ICASE = 1                                              000006
 00123    33*               IGAM = 0                                               000007
 00124    34*               DO 300 I=1,26                                          000013
 00127    35*               PCP(I)= 0.                                             000013
 00130    36*         300   SUBAR(I) = 0.0                                         000013
 00132    37*               EQL = .TRUE.                                           000015
 00133    38*               FROZ = .FALSE.                                         000017
 00134    39*               WRITE (6,302)                                          000020
 00136    40*         302   FORMAT (' BEGIN NAMELIST RKTINP INPUT')                000026
 00137    41*         303   READ (5,RKTINP)                                        000026
 00142    42*               NPP = 0                                                000031
 00143    43*               DO 305 I = 1,26                                        000035
 00146    44*               IF (PCP(I) .LE. 0.0)  GO TO 306                        000035
 00150    45*         305   NPP = I                                                000040
 00152    46*         306   NPP = NPP*2                                            000045
 00153    47*               NSUB = 0                                               000047
 00154    48*               NSUP = 0                                               000050
 00155    49*               DO 320  I=1,13                                         000054
 00160    50*               IF (SUBAR(I) .GT. 0.0)  NSUB = NSUB + 1                000054
 00162    51*         320   IF (SUPAR(I) .GT. 0.0)  NSUP = NSUP + 1                000061
 00165    52*               WRITE(JOUT,RKTINP)                                     000071
 00170    53*               SEQL = EQL                                             000075
 00171    54*               IOF = 0                                                000077
 00172    55*               II = 3000.                                             000100
 00172    56*       C       LOOP FOR EACH O/F                                      000100
 00173    57*         321   IT = 1                                                 000103
 00174    58*               IOF = IOF + 1                                          000104
 00175    59*               OF = OXF(IOF)                                          000107
 00176    60*               CALL NEWOF                                             000111
 00177    61*               IF (T(1) .LE. 0.0)  GO TO 322                          000113
 00201    62*               TT = T(IT)                                             000117
 00201    63*       C       LOOP FOR CHAMBER PRESSURES                             000117
 00202    64*         322   DO 998 IP = 1,NP                                       000122
 00205    65*               ITNUM = 0                                              000126
 00206    66*               AREA = .FALSE.                                         000127
 00207    67*               IF (T(1) .LE. 0.0)  HP = .TRUE.                        000130
 00211    68*               IF (T(1) .GT. 0.0)  TP = .TRUE.                        000135
 00213    69*               SP = .FALSE.                                           000142
 00214    70*               EQL = .TRUE.                                           000143
 00215    71*               ISUB = 1                                               000145
 00216    72*               ISUP = 1                                               000146
 00217    73*               PP = P(IP)                                             000147
 00220    74*               IPP = 1                                                000151
 00220    75*       C       LOOP FOR PRESSURE RATIOS                               000151
 00221    76*         331   IF(EQL)  GO TO 332                                     000153
 00223    77*               CALL FROZEN                                            000154
 00224    78*               GO TO 1332                                             000156
 00225    79*         332   CALL EQLBRM                                            000160
 00225    80*       C       TT = 0 IF NO CONVERGENCE                               000160
 00226    81*        1332   IF (TT .GT. 0.0)  GO TO 333                            000162
 00230    82*               IF (NPT .LT. 2)  RETURN                                000164
 00232    83*               GO TO 900                                              000173
 00233    84*         333   IF(IPP.GT.1) GO TO 195                                 000175
 00233    85*       C       COMBUSTION CHAMBER                       ROCK0060      000175
 00235    86*               EQL = SEQL                                             000200
 00236    87*               TP = .FALSE.                             ROCK0062      000202
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00237      88*          HP = .FALSE.                                                    ROCK0063     000203
00240      89*          SP = .TRUE.                                                     ROCK0064     000204
00241      90*          SO = SSUM(1)                                                                 000206
00242      91*          CPRF = CPSUM                                                                 000210
00243      92*     334  TMELT=0.                                                                     000213
00244      93*          ITROT = 3                                                                    000213
00245      94*          THI = .FALSE.                                                                000215
00246      95*          APP(2)=((GAMMAS(1)+1.)/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))          ROCK0066     000216
00247      96*          IF(EQL)  WRITE(JOUT,194) APP(2)                                              000234
00253      97*          PP = PPP(1)/APP(2)                                                           000244
00254      98*          TT = 2.*TT/(GAMMAS(1)+1.)                                                    000247
00255      99*          ISV = 1                                                                      000255
00256     100*          GO TO 870                                                                    000257
00257     101*     195  USQ = 2.0*RBR*(HSUM(1) - HSUM(NPT))                                          000261
00260     102*          IF (IPP.GT.2) GO TO 900                                                      000271
00260     103*    C     THROAT                                                          ROCK0073     000271
00262     104*          IF (.NOT. THI)  GO TO 191                                                    000275
00264     105*          GAMMAS(2) = 0.                                                               000277
00265     106*          GO TO 899                                                                    000300
00264     107*     191  ASQ = RBR*GAMMAS(2)*TT*ENN                                                   000302
00267     108*          IF(IDEBUG.EQ.1.OR.IDEBUG.EQ.2)  WRITE(JOUT,923)USQ,ASQ                       000311
00274     109*     923  FORMAT(5HOUSQ=,E15.8,5X,4HASQ=,E15.8)                                        000334
00275     110*          DH = (USQ-ASQ)/ASQ                                                           000334
00276     111*          IF(DH.LT.0.)  DH=-DH                                                         000341
00300     112*          IF(DH.LE.0.4E-4.OR.ITROT.EQ.0)  GO TO 899                                    000346
00302     113*          IF (JSOL .NE. 0)  GO TO 925                                                  000361
00304     114*          IF (TMELT .LE. 0.0)  GO TO 192                                               000363
00306     115*          DLT = ALOG(TMELT/TT)                                                         000366
00307     116*          PP = PP*EXP(DLT*CPR(2)/(ENN*DLVTP(2)))                                       000375
00310     117*          APP(2) = P(IP)/PP                                                            000407
00311     118*          THI = .TRUE.                                                                 000412
00312     119*          GO TO 331                                                                    000414
00313     120*     925  TMELT = TT                                                                   000416
00314     121*     192  APP(2) = APP(2)/(1.0 + (USQ - ASQ)/(ENN*(GAMMAS(2) + 1.0)*RBR*TT))           000420
00315     122*          PP = P(IP)/APP(2)                                                            000437
00316     123*          ITROT = ITROT-1                                                 ROCK0079     000442
00317     124*          IF(EQL)  WRITE(JOUT,194) APP(2)                                              000445
00323     125*     194  FORMAT(7H PC/PT=,F9.6)                                                       000455
00324     126*          GO TO 331                                                                    000455
00325     127*     899  AWT =ENN*TT/(PP*USQ**.5)                                                     000457
00326     128*          PCPLT = ALOG(APP(2))                                                         000472
00327     129*     900  ISV =0                                                                       000477
00330     130*          IF (TT .LE. 0.0)  GO TO 860                                                  000500
00332     131*          AEAT(NPT) = ENN*TT/(PP*USQ**.5*AWT)                                          000503
00333     132*          IF(AREA)  GO TO 800                                                          000521
00335     133*          IF(IPP.LT.NPP)  GO TO 859                                                    000523
00337     134*          IF((NSUB+NSUP).EQ.0)  GO TO 860                                              000527
00341     135*          AREA = .TRUE.                                                                000533
00341     136*    C     PCP ESTIMATES FOR AREA RATIOS                                                000533
00342     137*     800  IF(ITNUM.NE.0)  GO TO 810                                                    000536
00344     138*          DLNP = 1.                                                                    000541
00345     139*          ITNUM = 1                                                                    000543
00346     140*          ARATIO = SUBAR(ISUB)                                                         000545
00347     141*          IF(NSUB.LE.0)  ARATIO=SUPAR(ISUP)                                            000551
00351     142*          ELN = ALOG(ARATIO)                                                           000557
00352     143*          IF(NSUB.LE.0)  GO TO 799                                                     000563
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00354   144*          APPL = PCPLT/(SUBAR(ISUB)+(10.587*ELN**2+9.454)*ELN)                000566
00355   145*          IF(ARATIO.LT.1.09)  APPL =.9*APPL                                     000577
00357   146*          GO TO 859                                                            000606
00360   147*      799 IF(SUPAR(ISUP).LT.2.)  GO TO 805                                     000610
00362   148*          IF(ISUP.GT.1.AND.SUPAR(ISUP-1).GE.2.)  GO TO 802                     000614
00364   149*          APPL = GAMMAS(2)+ELN*1.4                                             000632
00365   150*          GO TO 859                                                            000636
00366   151*      805 APPL = SQRT(ELN*(1.535+3.294*ELN))+PCPLT                             000640
00367   152*          GO TO 859                                                            000651
00370   153*      810 IF (IDEBUG .LE. 0 .OR. NPT .LT. IDEBUG)  GO TO 809                   000653
00372   154*          WRITE(JOUT,1811) ITNUM,ARATIO,AEAT(NPT),APP(NPT),DLNP               000667
00401   155*     1811 FORMAT (6H0ITER=,I2,5X,15HASSIGNED AE/AT=,F15.8,5X,6HAE/AT=,F15.8,      000703
00401   156*         15X,5HPC/P=,F15.8,5X,11HDELTA LN P=,F15.8)                            000703
00402   157*      809 TOL = 1.0E-5                                                         000703
00403   158*          IF (ARATIO .GE. 10.0)  TOL = 4.0E-5                                  000706
00405   159*          IF (ABS(AEAT(NPT) - ARATIO)/ARATIO .LE. TOL)  GO TO 830              000714
00407   160*          IF (ABS(DLNP) .LT. 4.0E-6)  GO TO 830                                000724
00411   161*          AEATL= ALOG(AEAT(NPT))                                               000730
00412   162*          ITNUM = ITNUM + 1                                                    000736
00413   163*          IF (ITNUM .GT. 25)  GO TO 820                                        000741
00415   164*          ASQ = RBR*GAMMAS(NPT)*ENN*TT                                         000744
00416   165*          DLNPE = GAMMAS(NPT)*USQ/(USQ-ASQ)                                    000754
00417   166*      802 DLNP = DLNPE*ELN-DLNPE*AEATL                                         000763
00420   167*          APPL = APPL + DLNP                                                   000771
00421   168*          IF(ITNUM.EQ.1)  GO TO 859                                            000773
00423   169*          APP(NPT) = EXP(APPL)                                                 000776
00424   170*          PP = P(IP)/APP(NPT)                                                  001002
00425   171*          GO TO 331                                                            001005
00426   172*      820 WRITE(JOUT,821) ARATIO                                               001007
00431   173*      821 FORMAT (/10X,40HROCKET DID NOT CONVERGE FOR AREA RATIO =,F11.6/)     001015
00432   174*      830 ITNUM = 0                                                            001015
00433   175*          AEAT(NPT) = ARATIO                                                   001016
00434   176*          IF(NSUB.LE.0)  GO TO 834                                             001020
00436   177*          ISUB = ISUB+1                                                        001023
00437   178*          IF (ISUB .LE. NSUB)  GO TO 800                                       001026
00441   179*          ISUB = 1                                                             001031
00442   180*          NSUB = -NSUB                                                         001033
00443   181*          IF(ISUP.LE.NSUP)  GO TO 800                                          001035
00445   182*          GO TO 835                                                            001041
00446   183*      834 ISUP = ISUP+1                                                        001043
00447   184*          IF(ISUP.LE.NSUP)  GO TO 800                                          001045
00451   185*          ISUP = 1                                                             001050
00452   186*      835 AREA = .FALSE.                                                       001053
00453   187*          GO TO 860                                                            001053
00454   188*      859 ISV = NPT                                                            001055
00455   189*          IF(NPT.NE.13)  GO TO 870                               ROCK0088      001056
00457   190*      860 CALL RKTOUT (IGAM)                                                   001061
00460   191*          IF (TT .LE. 0.0)  ISV = 0                                            001063
00462   192*          IF (.NOT. EQL .AND. TT .LE. 0.0)  WRITE(JOUT,862)                    001067
00465   193*      862 FORMAT (//2X,125HCALCULATIONS WERE STOPPED IN ROCKET BECAUSE NEXT     001104
00465   194*         1POINT IS MORE THAN 50 DEGREES BELOW TEMPERATURE RANGE OF A CONDENS   001104
00465   195*         2ED SPECIES)                                                          001104
00466   196*          IF (ISV.EQ.0) GO TO 990                                              001104
00470   197*          IDEBUG = IDEBUG-13                                                   001106
00471   198*          WRITE(JOUT,865)                                                      001111
00473   199*      865 FORMAT(1H1)                                                          001116
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00474     200*          NPT = 2                                                   001116
00475     201*      870 NPT = NPT + 1                              ROCK0121       001121
00476     202*          IF(.NOT.EQL)  GO TO 880                                   001123
00500     203*          IF(ISV.EQ.1)  ISV = -1                                    001125
00502     204*          CALL SAVE                                                 001132
00503     205*      880 IPP = IPP+1                                               001136
00504     206*          IF(NPT.EQ.2)  GO TO 331                                   001140
00506     207*          IF(.NOT.AREA)  APP(NPT)=PCP(IPP-2)                        001143
00510     208*          IF(AREA)  APP(NPT)=EXP(APPL)                              001154
00512     209*          PP = P(IP)/APP(NPT)                                       001163
00513     210*          GO TO 331                                                 001167
00514     211*      990 IF(IDEBUG.LT.0)  IDEBUG=IDEBUG+13                         001171
00516     212*          IF(NSUB.LT.0)  NSUB=-NSUB                                 001176
00520     213*          IF (.NOT.FROZ.OR..NOT.EQL)  GO TO 997                     001203
00522     214*          CPR(1) = CPRF                                             001206
00523     215*          GAMMAS(1) = CPRF/(CPRF-1./WM(1))                          001210
00524     216*          TT = TTT(1)                                               001215
00525     217*          IPP = 1                                                   001217
00526     218*          NPT = 1                                                   001221
00527     219*          CALL SAVE                                                 001222
00530     220*          EQL = .FALSE.                                             001224
00531     221*          ENN = 1./WM(1)                                            001226
00532     222*          GO TO 334                                                 001230
00533     223*      997 NPT = 1                                                   001232
00534     224*          WRITE(JOUT,865)                                           001233
00536     225*          IF (SEQL)  CALL SAVE                                      001240
00540     226*      998 TT = TTT(1)                                               001244
00542     227*          IF(IT.GE.NT)  GO TO 999                                   001250
00544     228*          IT = IT+1                                                 001254
00545     229*          TT = T(IT)                                                001260
00546     230*          GO TC 322                                                 001262
00547     231*      999 IF (IOF .GE. NOF)  RETURN                                 001264
00551     232*          GO TO 321                                                 001272
00552     233*          END                                        ROCK0129       001316

      END OF COMPILATION:          NO  DIAGNOSTICS.

@HDG,P       RREAD
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@FOR,S    RREAD,RREAD
HSA 'E3 -10/15/80-13:07:40 (26,)

 SUBROUTINE RREAD      ENTRY POINT 001330

 STORAGE USED: CODE(1) 001345; DATA(0) 001373; BLANK COMMON(2) 000000

  COMMON BLOCKS:

  0003   CFVEL   000001

 EXTERNAL REFERENCES (BLOCK, NAME)

  0004    RDYES
  0005    PAGIT
  0006    CHRSIZ
  0007    GOUT
  0010    NNCOD$
  0011    RDATAI
  0012    RDATAF
  0013    DMWRIF
  0014    RDCHAR
  0015    NREW$
  0016    NRBU$
  0017    NIO2$
  0020    NIO1$
  0021    NERR2$
  0022    NWBU$
  0023    NWEF$
  0024    NERR3$

 STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

  0001     000014 10L       0001     000277 100L      0001     000375 106L      0001     000437 110L      0001     000517 120L
  0001     000551 130L      0001     000605 140L      0001     000623 150L      0001     000644 160L      0001     000662 170L
  0001     000041 176G      0001     000703 200L      0001     000045 2026      0001     000116 2326      0001     000134 242G
  0001     000747 300L      0001     001032 310L      0001     000326 3226      0001     001062 330L      0001     001110 340L
  0001     000366 344G      0001     001127 350L      0001     001144 360L      0001     000454 3656      0001     001163 370L
  0001     000501 376C      0001     001201 400L      0001     001216 408L      0001     001305 420L      0001     000716 4506
  0001     000717 453G      0001     000070 50L       0001     000770 501G      0001     001015 5126      0001     001210 565G
  0001     001231 602G      0001     001235 606G      0001     001276 635G      0001     000177 70L       0000     001276 802F
  0001     000240 90L       0001     000274 95L       0000 R 000226 ANUM      0003 R 000000 CF        0000 R 000702 DENS
  0000 R 000536 ENTH      0000 R 001125 EXMP1A    0000 R 001140 EXMP1B    0000 R 001150 EXMP2     0000 R 001156 EXMP2B
  0000 R 001163 EXMP3     0000 R 001170 EXMP3B    0000 R 001177 EXMP4     0000 R 001203 EXMP5     0000 R 001207 EXMP6
  0000 R 001214 EXMP7     0000 R 000567 FAZ       0000 R 000651 FOX       0000 I 001252 I         0000 I 001257 ICHNG
  0000   001347 INJPS     0000 I 001250 IO        0000 I 001255 IOPT      0000 I 001023 IOUT      0000 I 001220 IREACT
  0000 I 001253 J         0000 I 001236 LINE0     0000 I 000733 LINE1     0000 I 000760 LINE2     0000 I 001003 LINE3
  0000 I 001050 MODIFY    0000 I 001065 MODMEN    0000 I 000535 MOLE      0000 I 001256 N         0000 I 000000 NAME
  0000 I 001254 NAST      0000 I 001260 NDUMMY    0000 I 001251 NREAC     0000 I 001246 N3        0000 I 001247 N8
  0000 R 000454 PECWT     0000 R 001224 RDUM      0004 L 000000 RDYES     0000 R 000620 RTEMP
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00101     1*              SUBROUTINE RREAD(FIRST)                                            000000
00103     2*              LOGICAL FIRST,RDYES                                                000000
00103     3*     C                                                                           000000
00103     4*     C        USE MIPS INPUT ROUTINES TO READ REACTANT CARDS (STORE ON FILE 8)   000000
00103     5*     C                                                                           000000
00103     6*     C        DATA ARRAYS FOR REACTANT CARDS                                     000000
00104     7*           DIMENSION NAME(25,6),ANUM(25,6),PECWT(25),MOLE(25),ENTH(25),          000000
00104     8*          X   FAZ(25),RTEMP(25),FOX(25),DENS(25)                                 000000
00105     9*     C                                                                           000000
00105    10*              COMMON /CFUEL/CF                                                   000000
00105    11*     C        ARRAYS FOR DATA MENU'S                                             000000
00106    12*              DIMENSION LINE1(21),LINE2(19),LINE3(16),IOUT(21),MODIFY(13)        000000
00107    13*              DIMENSION MODMEN(4,8),EXMP1A(11),EXMP1B(8),EXMP2(6),EXMP2B(5),     000000
00107    14*          1   EXMP3(5),EXMP3B(7),EXMP4(4),EXMP5(4),EXMP6(5),EXMP7(4),            000000
00107    15*          2   IREACT(4),ROUM(10),LINED(8)                                        000000
00107    16*     C                                                                           000000
00107    17*     C        SET DATA ARRAYS FOR MENUS                                          000000
00110    18*              DATA LINED/6HTYPE  ,6HYES  T,6HO READ,6H IN PR,6HEVIOUS,           000000
00110    19*          1   6H REACT,6HANT SE,6HT      /                                       000000
00112    20*              DATA LINE1/6H INDEX,4*6H      ,6HREACTA,6HNT(*) ,3*6H      ,       000000
00112    21*          1   6H     R,6HEL WT/,6H  MOL,6HE  ENT,6HHALPY/,6H   PHA,6HSE  TE,     000000
00112    22*          2   6HMP,K  ,6H FUEL/,6H  DENS,6HITY   /                               000000
00114    23*              DATA LINE2/10*6H      ,6H     N,6HO MOLE,6HS     ,6H   INT,        000000
00114    24*          1   6H ENERG,6HY     ,2*6H      ,6H OXID /                             000000
00116    25*              DATA LINE3/8*6H      ,6H  *   ,6H   IND,6HICATES,6H ENTHA,         000000
00116    26*          1   6HLPY TO,6H BE CA,6HLCULAT,6HED      /                             000000
00120    27*              DATA MODMEN/24H 1-REACTANT FORMULA      ,                          000000
00120    28*          1   24H 2-REL WT/NO MOLES      ,24H 3-ENTHALPY/ENERGY//CALC ,          000000
00120    29*          2   24H 4-PHASE (S-L-G)        ,24H 5-TEMPERATURE (K)       ,          000000
00120    30*          3   24H 6-FUEL,OXIDIZER (F/O)  ,24H 7-DENSITY (G/CM3)       ,          000000
00120    31*          4   24H RETURN TO CONTINUE     /                                       000000
00122    32*              DATA EXMP1A/36H TYPE CHEMICAL FORMULA THIS REACTANT,               000000
00122    33*          1   30H, HOLLERINTH CODE FOR SYMBOLS /                                 000000
00124    34*             DATA EXMP1B/48H EXAMPLE CARBON TETRACHLORIDE  1HC 1. 2HCL 4.   /    000000
00126    35*              DATA EXMP2/36H TYPE REL WEIGHT/NUMBER OF MOLES    /                000000
00130    36*              DATA EXMP2B/30H TYPE YES IF VALUE IS MOLES   /                     000000
00132    37*              DATA EXMP3/30H TYPE ENTHALPY/INTERNAL ENERGY/                      000000
00134    38*              DATA EXMP3B/42H TYPE YES IF ENTHALPY TO BE CALCULATED    /         000000
00136    39*              DATA EXMP4/24H TYPE PHASE (S-L-G)     /                            000000
00140    40*              DATA EXMP5/24H TYPE TEMPERATURE (K)    /                           000000
00142    41*              DATA EXMP6/30H TYPE FUEL/OXIDIZER (F/O)     /                      000000
00144    42*              DATA EXMP7/24H TYPE DENSITY (G/CC)     /                           000000
00146    43*              DATA MODIFY/6H TYPE ,6H 1, 2,,6HOR 3  ,6HTO MOD,6HIFY, D,          000000
00146    44*          1   6HELETE,,6H OR AD,6HD A RE,6HACTANT,6H (RETU,6HRN TO ,             000000
00146    45*          2   6HCONTIN,6HUE)    /                                                000000
00150    46*              DATA IREACT/24H TYPE REACTANT NUMBER    /                          000000
00152    47*           DATA N3/8/,N8/12/                                                     000000
00152    48*     C                                                                           000000
00155    49*           CALL PAGIT                                                            000000
00156    50*              IO=N3                                                              000001
00157    51*         6    NREAC=0                                                            000003
00157    52*     C                                                                           000003
00157    53*     C        FOR FIRST PASS DO NOT CHECK SAVED DATA                             000003
00160    54*              IF(.NOT.FIRST) GO TO 10                                            000004
00162    55*              IF(.NOT.RDYES(LINED,43)) GO TO 50                                  000006
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00162    56*   C                                                                 000006
00162    57*   C         READ IN PRESENT CASE                                     000006
00164    58*    10       CONTINUE                                                 000014
00165    59*             IF (IO.EQ.N3) REWIND IO                                  000014
00167    60*             READ (IO) NREAC,CF                                       000021
00173    61*             IF(NREAC.LT.1) GO TO 50                                  000027
00175    62*             DO 25 I=1,NREAC                                          000033
00200    63*             READ (IO) (NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),  000041
00200    64*          X  ENTH(I),NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOX(I),DENS(I)   000041
00220    65*    25       CONTINUE                                                 000070
00220    66*   C                                                                  000070
00220    67*   C         DISPLAY PRESENT SET OF REACTANTS (ADD IF NONE EXIST)     000070
00222    68*    50       CONTINUE                                                 000070
00223    69*             CALL PAGIT                                               000070
00224    70*             CALL CHRSIZ(4)                                           000071
00225    71*          IF (NREAC.LT.1) GO TO 70                                    000074
00227    72*             CALL GOUT(LINE1,125)                                     000100
00230    73*             CALL GOUT(LINE2,119)                                     000104
00231    74*             DO 60 I=1,NREAC                                          000116
00234    75*             NAST=1H                                                  000116
00235    76*             IF (NAME(I,6).EQ.2H00) NAST=1H*                          000120
00237    77*             ENCODE(802,IOUT,1) (NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),   000125
00237    78*          X  ENTH(I),NAST,FAZ(I),RTEMP(I),FOX(I),DENS(I)              000125
00257    79*             CALL GOUT(IOUT,125)                                      000151
00260    80*    60       CONTINUE                                                 000162
00262    81*          CALL GOUT(' ',1)                                            000162
00263    82*             CALL GOUT(LINE3,92)                                      000166
00264    83*          CALL GOUT(' ',1)                                            000172
00265    84*    70       CONTINUE                                                 000177
00266    85*             CALL GOUT(MODIFY,75)                                     000177
00267    86*             IOPT=0                                                   000202
00270    87*             CALL RDATAI(1,IOPT,$70)                                  000203
00271    88*             IF(IOPT.LT.0 .OR. IOPT.GT.3) GO TO 70                    000210
00273    89*             IF(IOPT.EQ.0) GO TO 400                                  000225
00275    90*             GO TO(90,90,300),IOPT                                    000227
00275    91*   C                                                                  000227
00275    92*   C         SELECT REACTANT NUMBER                                   000227
00276    93*    90       CONTINUE                                                 000240
00277    94*             N=1                                                      000240
00300    95*             IF(NREAC.EQ.1) GO TO 95                                  000241
00302    96*             N=0                                                      000243
00303    97*             CALL GOUT(IREACT,24)                                     000244
00304    98*             CALL RDATAI(1,N,$90)                                     000250
00305    99*             IF(N.LT.1 .OR. N.GT.NREAC) GO TO 90                      000255
00307   100*    95       CONTINUE                                                 000274
00310   101*             IF(IOPT.EQ.2) GO TO 200                                  000274
00310   102*   C                                                                  000274
00310   103*   C         SELECT MODIFICATION OPTIONS                              000274
00312   104*   100       CONTINUE                                                 000277
00313   105*             CALL PAGIT                                               000277
00314   106*             NAST=1H                                                  000300
00315   107*             IF (NAME(I,6).EQ.2H00) NAST=1H*                          000302
00317   108*             ENCODE(802,IOUT)N,(NAME(N,J),ANUM(N,J),J=1,5),PECWT(N),MOLE(N),   000312
00317   109*          X  ENTH(N),NAST,FAZ(N),RTEMP(N),FOX(N),DENS(N)              000312
00337   110*             CALL GOUT(LINE1,125)                                     000343
00340   111*             CALL GOUT(LINE2,114)                                     000347
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00341   112*              CALL GOUT(IOUT,125)                          000353
00342   113*            CALL GOUT(' ',1)                               000357
00343   114*              DO 105 I=1,8                                 000366
00346   115*              CALL GOUT(MODMEN(1,I),24)                    000366
00347   116*      105     CONTINUE                                     000375
00351   117*      106     CONTINUE                                     000375
00352   118*              ICHNG=0                                      000375
00353   119*              CALL RDATAI(1,ICHNG,$106)                    000376
00354   120*              IF(ICHNG .EQ. 0) GO TO 50                    000402
00356   121*              IF(ICHNG.LT.1 .OR. ICHNG.GT.7) GO TO 106     000404
00360   122*              GO TO (110,120,130,140,150,160,170),ICHNG    000422
00361   123*      110     CONTINUE                                     000437
00362   124*              CALL GOUT(EXMP1A,66)                         000437
00363   125*              CALL GOUT(EXMP1B,48)                         000442
00364   126*              DO 112 I=1,5                                 000454
00367   127*              J=(I-1)*2 + 1                                000454
00370   128*              RDUM(J)=2H                                   000461
00371   129*              RDUM(J+1)=0.                                 000464
00372   130*      112     CONTINUE                                     000467
00374   131*              CALL RDATAF(10,RDUM,$110)                    000467
00375   132*              DO 114 I=1,5                                 000501
00400   133*              J=(I-1)*2 + 1                                000503
00401   134*              FLD(0,36,NAME(N,I))=FLD(0,36,RDUM(J))        000507
00401   135*      C     CALL CHECK(NAME(N,I))                          000507
00402   136*              ANUM(N,I)=RDUM(J+1)                          000511
00403   137*      114     CONTINUE                                     000515
00405   138*              GO TO 100                                    000515
00405   139*      C                                                    000515
00406   140*      120     CONTINUE                                     000517
00407   141*              CALL DMWRTF(EXMP2,36,PECWT(N),6)             000517
00410   142*              CALL RDATAF(1,PECWT(N),$120)                 000527
00411   143*              MOLE(N)=1H                                   000536
00412   144*              IF(.NOT.RDYES(EXMP2B,30)) GO TO 100          000540
00414   145*              MOLE(N)=1HM                                  000545
00415   146*              GO TO 100                                    000547
00415   147*      C                                                    000547
00416   148*      130     CONTINUE                                     000551
00417   149*              CALL DMWRTF(EXMP3,30,ENTH(N),5)              000551
00420   150*              CALL RDATAF(1,ENTH(N),$130)                  000561
00421   151*              NAME(N,6)=2H                                 000570
00422   152*              IF (RDYES(EXMP3B,42)) NAME(N,6)=2HOO         000573
00424   153*              GO TO 100                                    000603
00424   154*      C                                                    000603
00425   155*      140     CONTINUE                                     000605
00426   156*              CALL GOUT(EXMP4,24)                          000605
00427   157*              CALL RDCHAR(FAZ(N),1,1,$140)                 000611
00430   158*              GO TO 100                                    000621
00430   159*      C                                                    000621
00431   160*      150     CONTINUE                                     000623
00432   161*              CALL DMWRTF(EXMP5,24,RTEMP(N),$150)          000623
00433   162*              CALL RDATAF(1,RTEMP(N),$150)                 000633
00434   163*              GO TO 100                                    000642
00434   164*      C                                                    000642
00435   165*      160     CONTINUE                                     000644
00436   166*              CALL GOUT(EXMP6,30)                          000644
00437   167*              CALL RDCHAR(FOX(N),1,1,$160)                 000650
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00440     169*           GO TO 100                                                        000660
00440     169*     C                                                                      000660
00441     170*     170   CONTINUE                                                         000662
00442     171*           CALL DMWRTF(EXMP7,24,DENS(N),5)                                  000662
00443     172*           CALL RDATAF(1,DENS(N),$170)                                      000672
00444     173*           GO TO 100                                                        000701
00444     174*     C                                                                      000701
00444     175*     C     DELETE A REACTANT                                                000701
00445     176*     200   CONTINUE                                                         000703
00446     177*           NREAC=NREAC-1                                                    000703
00447     178*           DO 220 I=N,NREAC                                                 000707
00452     179*           DO 210 J=1,6                                                     000717
00455     180*                 NAME(I,J)=NAME(I+1,J)                                      000717
00456     181*                 ANUM(I,J)=ANUM(I+1,J)                                      000720
00457     182*     210   CONTINUE                                                         000723
00461     183*           PECWT(I)=PECWT(I+1)                                              000723
00462     184*           MOLE(I)=MOLE(I+1)                                                000725
00463     185*           ENTH(I)=ENTH(I+1)                                                000727
00464     186*           FAZ(I)=FAZ(I+1)                                                  000731
00465     187*           RTEMP(I)=RTEMP(I+1)                                              000733
00466     188*           FOX(I)=FOX(I+1)                                                  000735
00467     189*           DENS(I)=DENS(I+1)                                                000737
00470     190*     220   CONTINUE                                                         000745
00472     191*           GO TO 50                                                         000745
00472     192*     C                                                                      000745
00472     193*     C     ADD A REACTANT                                                   000745
00473     194*     300   CONTINUE                                                         000747
00474     195*           NREAC=NREAC+1                                                    000747
00475     196*           N=NREAC                                                          000751
00476     197*           CALL GOUT(EXMP1A,66)                                             000752
00477     198*           CALL GOUT(EXMP1B,48)                                             000756
00500     199*           DO 305 I=1,6                                                     000770
00503     200*           J=(I-1)*2 + 1                                                    000770
00504     201*           RDUM(J)=2H                                                       000775
00505     202*           RDUM(J+1)=0.                                                     001000
00506     203*     305   CONTINUE                                                         001003
00510     204*           CALL RDATAF(10,RDUM,$300)                                        001003
00511     205*           DO 307 I=1,5                                                     001015
00514     206*           J=(I-1)*2 + 1                                                    001015
00515     207*           FLD(0,36,NAME(N,I))=FLD(0,36,RDUM(J))                            001023
00515     208*     C     CALL CHECK(NAME(N,I))                                            001023
00516     209*           ANUM(N,I)=RDUM(J+1)                                              001025
00517     210*     307   CONTINUE                                                         001032
00521     211*     310   CONTINUE                                                         001032
00522     212*           CALL GOUT(EXMP2,36)                                              001032
00523     213*           PECWT(N)=0.                                                      001036
00524     214*           CALL RDATAF(1,PECWT(N),$310)                                     001037
00525     215*     320   CONTINUE                                                         001046
00526     216*           MOLE(N)=1H                                                       001046
00527     217*           IF(RDYES(EXMP2B,30)) MOLE(N)=1HM                                 001051
00531     218*     330   CONTINUE                                                         001062
00532     219*           CALL GOUT(EXMP3,30)                                              001062
00533     220*           ENTH(N)=0.                                                       001066
00534     221*           CALL RDATAF(1,ENTH(N),$330)                                      001067
00535     222*           IF (RDYES(EXMP3B,42)) NAME(N,6)=2H00                             001077
00537     223*     340   CONTINUE                                                         001110
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00540    224*              CALL GOUT(EXMP4,24)                                                        001110
00541    225*              FAZ(N)=1HS                                                                 001114
00542    226*              CALL RDCHAR(FAZ(N),1,-1,$340)                                              001116
00543    227*       350    CONTINUE                                                                   001127
00544    228*              CALL GOUT(EXMP5,24)                                                        001127
00545    229*              RTEMP(N)=0.                                                                001133
00546    230*              CALL RDATAF(1,RTEMP(N),$350)                                               001134
00547    231*       360    CONTINUE                                                                   001144
00550    232*              CALL GOUT(EXMP6,30)                                                        001144
00551    233*              FOX(N)=1HF                                                                 001150
00552    234*              CALL RDCHAR(FOX(N),1,-1,$360)                                              001152
00553    235*       370    CONTINUE                                                                   001163
00554    236*              CALL GOUT(EXMP7,24)                                                        001163
00555    237*              DENS(N)=0.                                                                 001167
00556    238*              CALL RDATAF(1,DENS(N),$370)                                                001170
00557    239*              GO TO 50                                                                   001177
00557    240*       C                                                                                 001177
00557    241*       C     STORE CASE TO FILE 8                                                       001177
00560    242*       400    CONTINUE                                                                   001201
00561    243*              REWIND IO                                                                  001201
00562    244*              IF (IO.NE.N8) GO TO 408                                                    001203
00564    245*              DO 406 I=1,5                                                               001210
00567    246*              READ (IO) NDUMMY                                                           001210
00572    247*       406    CONTINUE                                                                   001216
00574    248*       408    CONTINUE                                                                   001216
00575    249*              WRITE (IO) NREAC,CF                                                        001216
00601    250*              DO 410 I=1,NREAC                                                           001231
00604    251*              WRITE (IO) (NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),                  001231
00604    252*         X    ENTH(I),NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOX(I),DENS(I)                 001231
00624    253*       410    CONTINUE                                                                   001257
00626    254*              IF (IO.EQ.N8) GO TO 420                                                    001257
00630    255*              IF (.NOT.RDYES('TYPE YES TO EDIT COAL REACTANT DATA',35))                  001262
00630    256*         X       GO TO 420                                                               001262
00632    257*              IO=N8                                                                      001267
00633    258*              REWIND IO                                                                  001271
00634    259*              DO 412 I=1,5                                                               001276
00637    260*              READ (IO) NDUMMY                                                           001276
00642    261*       412    CONTINUE                                                                   001303
00644    262*            GO TO 10                                                                     001303
00645    263*       420    ENDFILE IO                                                                 001305
00646    264*              RETURN                                                                     001307
00647    265*       802 FORMAT(1X,I2,2X,5(A2,F8.4,2X),F10.6,2X,A1,F13.4,A1,3X,A1,F12.3,              001344
00647    266*         1    3X,A1,F12.5,1X)                                                            001344
00650    267*              END                                                                        001344

     END OF COMPILATION:        NO DIAGNOSTICS.

@HDG,P      SAVE
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@FOR,S    SAVE,SAVE
HSA  E3 -10/15/80-13:07:45 (13,1)

   SUBROUTINE SAVE        ENTRY POINT 000501
              NEWOF       ENTRY POINT 000504

   STORAGE USED: CODE(1) 000507; DATA(0) 000104; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003     CONSTS 000006
    0004     MOLCON 000010
    0005     SPECES 017106
    0006     MISC   001701
    0007     INDX   000041
    0010     CCC    000001
    0011     CFUEL  000004

   EXTERNAL REFERENCES (BLOCK, NAME)

    0012     MCALC
    0013     EXP
    0014     NWDU$
    0015     NIO2$
    0016     NIO1$
    0017     NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001     000137 100L     0001     000056 13L      0001     000042 132G     0001     000073 18L      0001     000112 20L
    0001     000172 200L     0001     000161 201G     0001     000207 210G     0001     000326 252G     0001     000241 302L
    0001     000435 317G     0001     000127 50L      0000     000014 730F     0000     000017 732F     0001     000311 744L
    0001     000322 745L     0001     000356 750L     0001     000365 760L     0000     000035 770F     0000     000045 780F
    0000     000050 785F     0005     011052 A        0006     000640 AM       0006     000705 AM1      0006     001135 ANUM
    0003     000000 ATMN     0006     000004 ATOM     0006 R   000514 BO       0006 R   000545 JMP      0007 L   000036 CALCH
    0011 R   000000 CT       0005     000000 COEF     0000 R   000006 COF      0007     000001 CONVG    0006     000706 CPR1
    0006     000634 CPSUM    0006     000654 DATA     0005     010624 DELN     0010     000002 DEMAND   0006     001560 DENS
    0005 R   004312 EN       0004     000000 END      0005 R   010150 ENLN     0006 R   001700 ENLSAV   0006 R   000000 ENN
    0006 R   001676 ENNL     0006 R   001677 ENSAVE   0006     001414 ENTH     0006 R   000636 EORAT    0006     001445 FAZ
    0000 R   000003 FCAL     0000 R   000013 FF       0000 R   000002 FHH      0006     001527 FOX      0000 R   000001 FUU
    0004     000001 GAS      0003     000001 GMET     0010     000000 GRAPH    0011     000001 HHVV     0007     000003 HP
    0006 R   000642 HFP      0000 R   000012 HS       0006 R   000637 HSUBO    0005     010376 HO       0007 I   000030 IC
    0007     000000 IDEBUG   0004 I   000002 IE       0007     000015 IMAT     0000     000057 INJP$    0007 L   000023 IONS
    0007     000021 IP       0007 I   000037 IQSAVE   0007 I   000016 IO1      0007 I   000005 ISV      0007     000034 IT
    0005 I   016266 IUSE     0004     000003 IZERO    0000 I   000005 J        0007 I   000026 JLIQ     0010 I   000001 JOUT
    0007 I   000025 JSOL     0007     000031 JS1      0007     000014 KMAT     0004 I   000004 LANK     0006 I   000463 LLMT
    0000 I   000004 LL1      0007 I   000040 LSAVE    0004     000005 MOL      0007     000006 MOLES    0006     000707 NAMF
    0007     000024 NC       0007     000022 NEWR     0007     000035 NFZ      0007 I   000012 NLM      0007     000017 NCF
    0007     000020 NOMIT    0007     000007 NP       0007 I   000011 NPT      0007     000027 NREAC    0007 I   000013 NS
    0000 I   000000 NSPP1    0007     000010 NT       0006 R   000635 OF       0004     000006 OX       0006     001644 OXF
    0003     000002 PATM     0006     001363 PFCMT    0011 R   000003 PER      0006     000633 PP       0003 R   000003 RBAR
    0003     000004 RER      0006 R   000644 RH       0006 R   001611 RHOP     0006     001612 RHW      0006     001476 RTEMP
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0003   000005 RVR      0005   004064 S        0007   000333 SHOCK    0005 R 016660 SLN      0007   000004 SP
0005   015369 SUB      0000 R 000007 SUM      0006   000001 SUMN     0006   000003 SO       0005   016814 TEMP
0006   000632 THIGH    0006   001643 TLN      0006   000630 TLOW     0006   000627 TM       0006   000631 TMID
0007   000002 TP       0006   000002 TT       0006 R 000646 VMIN     0007 L 000032 VOL      0006 R 000650 VPLS
0000 R 000011 V1       0000 R 000010 V2       0011 R 000002 WCR      0006   000652 WP       0004   000007 ZERO


00101      1*          SUBROUTINE SAVE                                                            000000
00101      2*    C                                                                                000000
00101      3*    C  SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES           000000
00101      4*    C                                                                                000000
00103      5*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                  /CONSTS/     000000
00104      6*          COMMON /MOLCON/ ENO,GAS,IE,IZERO,LANK,MOL,OX,ZERO            /MOLCON/     000000
00104      7*    C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),MO(150)            000000
00104      8*    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150),            000000
00105      9*          INCLUDE SPECPK                                                             000000
00111     10*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                  000000
00111     11*         1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,              000000
00111     12*         2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),   /MISC/     000000
00111     13*         3              DATA(25),AMI,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),           000000
00111     14*         4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,            000000
00111     15*         5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                       000000
00112     16*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,  /INDX/   000000
00112     17*         1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/   000000
00112     18*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE   /INDX/    000000
00112     19*    C                                                                                000000
00113     20*             COMMON /CCC/ GRAPH,JOUT,DEMAND                                          000000
00114     21*          COMMON /CFUEL/CF,MMVV,WCR,PER                                              000000
00114     22*    C                                                                                000000
00115     23*          DATA FUU/4HU, C/,FMM/4HM, C/,FCAL/4HAL/8/                                  000000
00121     24*          LOGICAL CALCH,IONS,VOL                                                     000000
00121     25*    C                                                                                000000
00122     26*          IF(ISV)100,10,200                                                          000000
00122     27*    C  NEXT POINT FIRST T IN SCHEDULE, USE PREVIOUS COMPOSITIONS FOR THIS T          000000
00125     28*       10 IQ1 = IQSAVE                                                               000003
00126     29*          ENN = ENSAVE                                                               000005
00127     30*          ENNL = ENLSAV                                                              000007
00130     31*          LL1 = NLM                                                                  000011
00131     32*          DO 50 J = 1,NS                                                             000042
00134     33*          IF (.NOT. IONS .OR. LLMT(NLM) .EQ. LSAVE)  GO TO 15                        000042
00136     34*          IF(LLMT(NLM).EQ.IE)  GO TO 13                                              000043
00140     35*          IF(IUSE(J).NE.-10000)  GO TO 15                                            000046
00142     36*          IUSE(J) = 0                                                                000051
00143     37*          LL1  = NLM+1                                                               000052
00144     38*          GO TO 20                                                                   000054
00145     39*       13 IF(SLN(J).NE.0..OR.IUSE(J).NE.0)  GO TO 15                                 000056
00147     40*          LL1 = NLM-1                                                                000065
00150     41*          IUSE(J) = -10000                                                           000067
00151     42*          GO TO 50                                                                   000071
00152     43*       15 IF (IUSE(J).EQ.0) GO TO 20                                                 000073
00154     44*          EN (J,NPT) = SLN(J)                                                        000074
00155     45*          IF(IUSE(J).GT.0) IUSE(J) = - IUSE(J)                                       000076
00157     46*          IF (EN(J,NPT) .GT. 0.0)  IUSE(J) = - IUSE(J)                               000103
00161     47*          GO TO 50                                                                   000110
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00162      48*        20 EN(J,NPT) = 0.                                                   000112
00163      49*           ENLN(J) = SLN(J)                                                 000112
00164      50*           IF (ENLN(J) + 18.50 .LE. ENNL)  GO TO 50                         000114
00166      51*           EN(J,NPT) = EXP(ENLN(J))                                         000120
00167      52*        50 CONTINUE                                                         000131
00171      53*           NLM = LL1                                                        000131
00172      54*           RETURN                                                           000133
00172      55*     C  FIRST T--SAVE COMPOSITIONS FOR FUTURE POINTS WITH THIS T            000133
00173      56*      100  ISV = -ISV                                                       000137
00174      57*           IQSAVE = IQ1                                                     000140
00175      58*           ENNSAVE = ENN                                                    000142
00176      59*           ENLSAV = ENNL                                                    000144
00177      60*           LSAVE = LLMT(NLM)                                                000146
00200      61*           DO 150 J = 1,NS                                                  000161
00203      62*           SLN(J) = ENLN(J)                                                 000161
00204      63*      150  IF (IUSE(J) .NE. 0)  SLN(J) = EN(J,ISV)                          000162
00204      64*     C  USE COMPOSITIONS FROM PREVIOUS POINT                                000162
00207      65*      200  DO 300 J = 1,NS                                                  000172
00212      66*      300  EN(J,NPT) = EN(J,ISV)                                            000207
00214      67*           RETURN                                                           000211
00214      68*     C  CALCULATE NEW VALUES OF BO AND HSUBO FOR NEW OF RATIO               000211
00215      69*           ENTRY NEWOF                                                      000214
00216      70*           WRITE(JOUT,730) OF                                               000214
00221      71*       730 FORMAT(6HCOF = ,F10.6)                                           000222
00222      72*           IF (CF+1.0) ,302,                                                000222
00225      73*           COF=OF/CF                                                        000225
00226      74*           WRITE (JOUT,732) COF,WCR,PER                                     000230
00233      75*       732 FORMAT (21X,'OXIDIZER/COAL=',F8.4,5X,'WATER/COAL=',F8.4,         000241
00233      76*          X    5X,'CARBON CONVERSION=',F8.4)                                000241
00234      77*       302 CONTINUE                                                         000241
00235      78*           SUM = OF + 1.                                                    000241
00236      79*           V2 =    (OF*VMIN(1)+VMIN(2))/SUM                                 000243
00237      80*           V1 =    (OF*VPLS(1)+VPLS(2))/SUM                                 000250
00240      81*           IF (V2 .LT. 0.0)  EQRAT = ABS(V1/V2)                             000255
00242      82*           IF (RH(1) .GT. 0.0 .AND. RH(2) .GT. 0.0)  GO TO 744              000264
00244      83*           RHOP = RH(2)                                                     000300
00245      84*           IF (RHOP .LE. 0.0)  RHOP = RH(1)                                 000302
00247      85*           GO TO 745                                                        000307
00250      86*       744 RHOP =  (OF+1.)*RH(1)*RH(2)/(RH(1)+ OF *RH(2))                   000311
00251      87*      745  DO 747 J = 1,NLM                                                 000322
00254      88*      747  BO(J) = (BOP(J,2) + BOP(J,1)*OF)/SUM                             000326
00256      89*           NPT = 1                                              MAIN0139    000333
00257      90*           IF(.NOT.CALCH)  GO TO 750                                        000335
00261      91*           CALL HCALC                                                       000337
00262      92*           CALCH = .FALSE.                                                  000341
00263      93*           IF (OF .GT. 0.0)  HPP(1) = SUM*HPP(1)/OF                         000342
00265      94*           HPP(2) = SUM*HPP(2)                                              000351
00266      95*           GO TO 760                                                        000354
00267      96*      750  HSUBO = (HPP(2) + HPP(1)*OF)/(RBAR*SUM)                          000356
00270      97*       760 IC = 0                                                           000365
00271      98*           JSOL = 0                                                         000365
00272      99*           JLIQ = 0                                                         000366
00273     100*           HS = RBAR*HSUBO                                                  000367
00274     101*           WRITE(JOUT,770)                                                  000372
00276     102*       770 FORMAT (1H0,17X,4HFUEL ,13X,7HOXIDANT  ,12X,7HMIXTURE  //)   MAIN0124    000377
00277     103*       780 FORMAT (1H 2A4,3E18.8/)                                      MAIN012     000377
```

```
00300    104*          FF = FHH                                                        000377
00301    105*          IF(VOL)FF = FUU                                                 000401
00303    106*          WRITE(JOUT,780) FF,FCAL ,HPP(2),HPP(1),HS                       000405
00312    107*          WRITE(JOUT,785)                                                 000421
00314    108*      785 FORMAT (12H KG-ATOMS/KG)                                        000426
00315    109*          WRITE(JOUT,790) (LLMT(J),LANK,BOP(J,2),BOP(J,1),BOL(J), J = 1,NLM)  000426
00327    110*          RETURN                                                          000444
00330    111*          END                                                             000506

      END OF COMPILATION:        NO  DIAGNOSTICS.

@HDG,P       SEARCH
```

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 @FOR,S    SEARCH,SEARCH
 HSA  E3 -10/15/80-13:07:48 (16,)

   SUBROUTINE SEARCH     ENTRY POINT 000445

   STORAGE USED: CODE(1) 000461; DATA(0) 000121; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003     HOLCON  000010
    0004     SPECES  017106
    0005     MISC    001701
    0006     INDX    000041
    0007     CCC     000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0010     MOVABS
    0011     HOLDIT
    0012     PAGIT
    0013     GOUT
    0014     NREW$
    0015     NRDU$
    0016     NIO2$
    0017     NIO1$
    0020     NWDU$
    0021     NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000     000022 10F        0001     000021 125G       0001     000022 130G       0001     000310 145L       0001     000050 146G
    0001     000102 154G       0001     000313 170L       0001     000125 171G       0001     000326 171L       0000     000045 172F
    0001     000126 173G       0000     000055 176F       0000     000030 20F        0001     000144 204G       0001     000154 207G
    0001     000204 220G       0001     000211 225G       0001     000222 233G       0001     000276 254G       0001     000346 277G
    0001     000376 306G       0000     000020 5F         0001     000042 7L         0001     000167 805L       0001     000171 810L
    0001     000225 820L       0001     000234 825L       0000     000032 871F       0004 R 011052 A           0005     000640 AM
    0005     000705 AM1        0005     001135 ANUM       0005     000004 ATOM       0000 R 000001 B           0005     000514 BO
    0005     000545 BOP        0006     000036 CALCH      0004 R 000000 COEF       0006     000001 CONVG      0005     000706 CPR1
    0005     000634 CPSUM      0005     000654 DATA       0004 R 004312 DATE       0004     010624 DELN       0007     000002 DEMAND
    0005     001560 DENS       0004     004312 EN         0003 I 000000 END        0004     010150 ENLN       0005     001700 ENLSAV
    0005     000000 ENN        0005     001676 ENNL       0005     001677 ENSAVE     0005     001414 ENTH       0005     000636 EQRAT
    0005     001445 FAZ        0005     001527 FOX        0003 I 000001 GAS        0007     000000 GRAPH      0006     000003 HP
    0005     000642 HPP        0005     000637 HSUBO      0004     010376 HO         0000 I 000013 I          0006     000030 IC
    0006     000000 IDEBUG     0003     000002 IE         0006     000015 IMAT       0000     000073 INJP$      0006     000023 IONS
    0006     000021 IP         0006     000037 IOSAVE     0006     000016 IO1        0006     000005 ISV        0006     000034 IT
    0004 I 016266 IUSE        0000 I 000012 IX          0003     000003 IZERO      0000 I 000014 J          0006     000026 JLIO
    0007 I 000001 JOUT        0006     000025 JSOL       0006     000031 JS1        0000 I 000017 K          0006     000014 KMAT
    0006 I 000012 L           0003     000004 LANK       0005 I 000463 LLMT       0006     000040 LSAVE      0003     000005 MOL
    0006     000006 MOLES      0000 I 000005 MT          0005     000707 NAME       0006 I 000024 NC         0006 L 000022 NEWR
    0006     000035 NFZ        0006     000017 NOF        0006 I 000020 NOMIT      0006     000007 NP         0006     000011 NPT
    0006     000027 NREAC      0006 I 000013 NS          0000 I 000000 NSPP1      0006     000010 NT         0005     000635 OF
    0004 I 010150 OMIT        0003     000006 OX         0005     001644 OXF       0005     001363 PECWT      0000 I 000011 PHAZ
```

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0005    000633 PP         0005    000644 RH         0005    001611 RHOP       0005    001612 RMW        0005    001476 RTEMP
0004    004064 S          0006    000033 SHOCK      0004    016660 SLN        0006    000004 SP         0004  I 015364 SUB
0005    000001 SUMN       0005    000003 SO         0004  R 016514 TEMP       0005  R 000632 THIGH      0005    001643 TLN
0005  R 000630 TLOW       0005    000627 TM         0005  R 000631 TMID       0006    000002 TP         0005    000002 TT
0000  R 000015 T1         0000  R 000016 T2         0005    000646 VMIN       0006    000032 VOL        0005    000650 VPLS
0005    000652 WP         0001    000007 ZERO
```

```
00101      1*            SUBROUTINE SEARCH                                                       000000
00101      2*      C                                                                             000000
00101      3*      C  SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED                   000000
00101      4*      C                                                                             000000
00103      5*            COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO              /HOLCON/  000000
00103      6*      C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)          000000
00103      7*      C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)           000000
00104      8*              INCLUDE SPECPK                                                        000000
00110      9*            COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),B0(25),               000000
00110     10*           1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,            000000
00110     11*           2              HSUB0,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),   /MISC/   000000
00110     12*           3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),         000000
00110     13*           4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,          000000
00110     14*           5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                     000000
00111     15*            COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,WP,NT,NPT,L,NS,   /INDX/   000000
00111     16*           1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ, /INDX/  000000
00111     17*           2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE   /INDX/  000000
00111     18*      C                                                                             000000
00112     19*               COMMON /CCC/ GRAPH,JOUT,DEMAND                                       000000
00112     20*      C                                                                             000000
00113     21*            DIMENSION B(4),DATE(2,3),MT(4),OMIT(3,3)                                000000
00114     22*            EQUIVALENCE (DATE,EN),(ENLN,OMIT)                                       000000
00115     23*            INTEGER END,GAS,OMIT,PHAZ,SUB                                           000000
00116     24*            LOGICAL NEWR                                                            000000
00116     25*      C                                                                             000000
00116     26*      C     CHANGE WHEN CHANGE SPECIES SIZE                                         000000
00117     27*            NSPP1=150                                                               000000
00120     28*            NC= 0                                                                   000001
00121     29*            IX= 0                                                                   000002
00122     30*            SUB(1,1) = END                                                          000003
00123     31*            REWIND 4                                                                000011
00124     32*            DO 3 I=1,150                                                            000022
00127     33*            DO 3  J=1,L                                                             000022
00132     34*         3  A(J,I) = 0.0                                                            000022
00135     35*            READ(4,5)  TLOW,TMID,THIGH                                              000027
00142     36*          5 FORMAT (3F10.3)                                                         000037
00143     37*            NS = 1                                                                  000037
00144     38*          7 READ     (4,10)(SUB(NS,I),I=1,3),DATE(1,NS),DATE(2,NS),(MT(J),B(J),      000042
00144     39*           1  J=1,4),PHAZ,T1,T2                                                     000042
00164     40*         10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3)                                 000112
00165     41*            IF(SUB(NS,1).EQ.END) GO TO 171                                          000112
00167     42*            READ     (4,20) ((COEF(I,J,NS),J=1,7),I=1,2)                            000115
00200     43*         20 FORMAT (5E15.8)                                                         000135
00201     44*            IF(NOMIT.EQ.0) GO TO 810                                                000135
00203     45*            DO 805 I=1,NOMIT                                                        000137
00206     46*            DO 808 J=1,3                                                            000154
```

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00211      47*     804  IF (OMIT(J,I) .NE. SUB(NS,J))  GO TO 805                          000154
00214      48*          GO TO 7                                                           000165
00215      49*      805 CONTINUE                                                          000171
00217      50*      810 DO 820 K=1,4                                                      000171
00222      51*          IF(B(K).EQ.0.) GO TO 825                                          000204
00224      52*          DO 168 I=1,L                                                      000211
00227      53*     168  IF (LLMT(I) .EQ. MT(K))  GO TO 820                                000211
00232      54*          DO 819 J=1,L                                                      000222
00235      55*      819 A(J,NS) = 0.                                                      000222
00237      56*          GO TO 7                                                           000223
00240      57*      820 A(I,NS)= B(K)                                                     000225
00242      58*      825 IUSE(NS) = 0                                                      000234
00243      59*          IF(PHAZ.EQ.GAS) GO TO 170                                         000235
00245      60*          NC= NC+1                                                          000240
00246      61*          TEMP(NC,1)= T1                                                    000243
00247      62*          TEMP(NC,2)= T2                                                    000246
00250      63*          IX= IX+1                                                          000250
00251      64*          IF(IUSE(NS-1).EQ.0 .OR. NC.EQ.1) GO TO 145                        000263
00253      65*          DO 830 I=1,L                                                      000276
00256      66*     830  IF (A(I,NS) .NE. A(I,NS-1))  GO TO 145                            000276
00261      67*          IX= IX-1                                                          000304
00262      68*      145 IUSE(NS)= -IX                                                     000310
00263      69*      170 NS= NS+1                                                          000313
00264      70*          IF (NS.LE.NSPP1) GO TO 7                                          000315
00266      71*          WRITE (JOUT,871)                                                  000320
00270      72*     871  FORMAT (//20X,54HDIMENSIONS IN /SPECES/ FOUND TO BE TOO SMALL IN S 000326
00270      73*         1EARCH/)                                                           000326
00271      74*      171 NS= NS-1                                                          000326
00272      75*          NEWR= .FALSE.                                                     000330
00273      76*          WRITE(JOUT,172)                                                   000335
00275      77*      172 FORMAT(42HOSPECIES BEING CONSIDERED IN THIS SYSTEM    )           000346
00276      78*          DO 174 I=1,NS,5                                                   000346
00301      79*          K = I + 4                                                         000351
00302      80*          IF (NS .LT. K)  K = NS                                            000354
00304      81*     174  WRITE(JOUT,176)(DATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),   000362
00304      82*         1   J=I,K)                                                         000362
00317      83*      176 FORMAT(5(5X,2A3,2X,3A4))                                          000407
00320      84*          CALL MOVABS(500,50)                                               000407
00321      85*          CALL HOLDIT                                                       000413
00322      86*          CALL PABIT                                                        000415
00323      87*          CALL GOUT(' ',1)                                                  000417
00324      88*          RETURN                                                            000423
00325      89*          END                                                               000460

    END OF COMPILATION:         NO  DIAGNOSTICS.

@HDG,P       SHCK
```

```
@FOR,S     SHCK,SHC
HSA  E3 -10/15/80-13:07:51 (12,)

    SUBROUTINE SHCK      ENTRY POINT 001367

    STORAGE USED: CODE(1) 001401; DATA(0) 000263; BLANK COMMON(2) 000000

     COMMON BLOCKS:

      0003    CONSIS 000006
      0004    HOLCON 000010
      0005    POINTS 000335
      0006    SPECES 017106
      0007    MISC   001701
      0010    DOUBLE 001560
      0011    INDX   000041
      0012    PERF   000166
      0013    OUPT   000073
      0014    CCC    000003

    EXTERNAL REFERENCES (BLOCK, NAME)

      0015    RDYES
      0016    PAGIT
      0017    CHRSIZ
      0020    GOUT
      0021    NEWOF
      0022    HCALC
      0023    OUT1
      0024    OUT2
      0025    EQLBRM
      0026    SAVE
      0027    OUT3
      0030    NWNLS
      0031    NRNLS
      0032    NWDUS
      0033    NIO2S
      0034    SQRT
      0035    NIO3S
      0036    NIO1S
      0037    ALOG
      0040    EXP
      0041    NERR3S

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

      0000    000143 125F      0001    000211 14L       0001    000011 145G      0001    000221 15L       0001    001001 150L
      0000    000165 152F      0001    000022 156G      0000    000101 16F       0001    001112 161L      0001    000126 17L
      0001    000143 19L       0001    000073 204G      0001    000114 21L       0001    000136 223G      0001    000147 231G
      0001    000245 30L       0001    000356 323G      0001    000376 334G      0001    000520 361G      0001    000534 40L
      0001    001125 431L      0001    000320 44L       0001    000325 45L       0000    000137 46F       0001    001057 461G
      0001    000412 47L       0001    000547 50L       0001    001201 520G      0001    001232 536G      0001    001247 547G
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0001   001266 5616     0001   001303 5726     0000   000176 58F      0001   001322 6046     0001   001345 6206
0000   000202 68F      0001   000750 75L      0000   000111 861F     0000   000122 862F     0000   000131 863F
0001   001106 88D      0006   011052 A        0007   000640 AM       0007 R 000705 AM1      0007   001135 ANUM
0003   000000 ATMN     0007   000004 ATOM     0000 R 000036 AX       0000 R 000037 AXX      0000 R 000024 A1
0007   000514 80       0007   000545 80P      0011   000036 CALCH    0006   000000 COEF     0011   000001 CONVG
0005 R 000032 CPR      0007 R 000706 CPR1     0007   000634 CPSUM    0007   000654 DATA     0006   010624 DELN
0014   000002 DEMAND   0007   001560 DENS     0005 R 000064 DLVPT    0005 R 000047 DLVTP    0006 R 004312 EN
0004   000000 END      0006 R 010150 ENLN     0007   001700 ENLSAV   0007   000000 ENN      0007   001676 ENNL
0007   001677 ENSAVE   0007   001414 ENTH     0012 L 000165 EOL      0007   000636 EQRAT    0013   000002 FA
0013   000003 FAP      0007   001445 FAZ      0013 R 000005 FB       0013   000006 FC       0013   000007 FCP
0013   000012 FCST     0013   000014 FCV      0013   000015 F6       0013   000017 F6E      0013   000020 F6V
0013   000021 FH       0013   000023 FI       0013   000025 FIV      0013   000027 FM       0000 R 000001 FMM
0013 R 000031 FMT      0013 R 000050 FN       0013 R 000052 FOUR     0007   001527 FOX      0013   000053 FP
0000 R 000002 FPP      0000 R 000003 FRA      0000 R 000004 FRB      0013   000054 FS       0013   000056 FSV
0013   000057 FT       0013   000061 FTK      0000 R 000005 FTT      0000 R 000006 FU1      0000 R 000007 FU2
0013   000063 FV       0013 R 000065 FVEL     0000 R 000010 FV21     0000 R 000011 FV22     0000 R 000012 FV23
0013 R 000001 F13      0013   000000 F9X      0010 D 000000 G        0005 R 000101 GAMMAS   0000 R 000020 GAMMA1
0004   000001 GAS      0010 D 001516 GG       0003   000001 GMET     0014   000000 GRAPH    0011   000003 HP
0007   000642 HPP      0000 R 000030 HS       0007 R 000637 HSUBO    0005 R 000000 HSUM     0006   010376 HO
0000 I 000022 I        0011   000030 IC       0011 I 000000 IDEBUG   0004   000002 IE       0011   000015 IMAT
0000 L 000013 INCDEQ   0000 L 000014 INCDFZ   0000   000233 INJPS    0000 I 000021 IOF      0011   000023 IONS
0011   000021 IP       0011   000037 IQSAVE   0011   000016 IQ1      0011 I 000005 ISV      0011   000034 IT
0006 I 016266 IUSE     0004 I 000003 IZERO    0000 I 000025 J        0011   000026 JLIQ     0014 I 000001 JOUT
0011   000025 JSOL     0011   000031 JS1      0000 I 000040 K        0011   000014 KMAT     0004   000004 LANK
0007   000463 LLMT     0011   000040 LSAVE    0012 R 000116 MACH1    0004   000005 MOL      0011   000006 MOLES
0000 R 000017 MU12RT   0000 R 000016 M1       0012 R 000150 M2M1     0007 I 000707 NAME     0011   000024 NC
0011   000022 NEWR     0011   000035 NFZ      0011   000012 NLM      0011 I 000017 NOF      0011   000020 NOMIT
0011   000007 NP       0011 I 000011 NPT      0011 I 000027 NREAC    0011 I 000013 NS       0000 I 000023 NSK
0000 I 000000 NSPP1    0011   000010 NT       0007 R 000635 OF       0013   000067 ONE      0004   000006 OX
0007 R 001644 OXF      0005 R 000116 P        0003   000002 PATM     0012 R 000000 PCP      0007   001363 PECWT
0007 R 000633 PP       0005 R 000217 PPP      0000 R 000026 P1       0000 R 000031 P21      0000 R 000033 P21L
0003   000003 RBAR     0003 R 000004 RBR      0015 L 000000 RDYES    0007   000644 RH       0007   001611 RHOP
0000 R 000035 RHO12    0007   001612 RMW      0012 R 000133 RRHO     0007 R 001476 RTEMP    0003   000005 RVR
0006   004064 S        0000 L 000015 SEQL     0000   000041 SHKINP   0011   000033 SHOCK    0006   016660 SLN
0005   000251 SONVEL   0011   000004 SP       0005 R 000015 SSUM     0006   015364 SUB      0007   000001 SUMN
0007   000003 SQ       0005 R 000150 T        0006   016514 TEMP     0007   000632 THIGH    0013 R 000070 THREE
0007 R 001643 TLN      0007   000630 TLOW     0007   000627 TM       0007   000631 TMID     0005   000320 TOTN
0011 L 000002 TP       0007 R 000002 TT       0005 R 000266 TTT      0013 R 000071 TWO      0000 R 000027 T1
0012 R 000047 T2T1     0000 R 000032 T21      0000 R 000034 T21L     0005 R 000303 UTWO     0012 R 000101 U1
0012 R 000064 U1U2     0005   000202 V        0007   000646 VMIN     0012   000032 VMOC     0011   000032 VOL
0007   000650 VPLS     0005 R 000234 WM       0007   000652 WP       0010 D 001510 X        0004   000007 ZERO
0013   000072 ZEROF
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```
00101      1*          SUBROUTINE SHCK                                                          000000
00101      2*    C                                                                              000000
00103      3*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                    /CONSTS/  000000
00104      4*          COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO              /HOLCON/  000000
00105      5*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)              000000
00105      6*         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)         000000
00105      7*         2 ,UTWO(13),TOTN(13)                                                      000000
00105      8*    C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)         000000
00105      9*    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)          000000
00106     10*          INCLUDE SPECPK                                                           000000
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00112          COMMON /MISC/ FNN,SUMN,TT,SD,ATOM(3,101),LLMT(25),BO(25),           000000
00112         1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,         000000
00112         2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),  /MISC/ 000000
00112         3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),      000000
00112         4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,       000000
00112         5              RMW(25),ILM,OXF(26),EMML,EMSAVE,EMLSAV                  000000
00113          COMMON /DOUBLE/ G(20,21), X(20)                                       000000
00114          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS, /INDX/ 000000
00114         1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/ 000000
00114         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE   /INDX/ 000000
00115          COMMON /PERF/ PCP(26),VMOC(13),T2T1(13),U1U2(13),U1(13),       /PERF/ 000000
00115         1              MACH1(13),RRHO(13),M2M1(13),EQL                   /PERF/ 000000
00116          COMMON /OUPT/ FOX,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),  /OUPT/ 000000
00116         1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/ 000000
00116         2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE, /OUPT/ 000000
00116         3              TWO,ZEROF                                         /OUPT/ 000000
00116    C                                                                           000000
00117             COMMON /CCC/ GRAPH,JOUT,DEMAND                                     000000
00117    C                                                                           000000
00120          DATA FMM/6HM2/M1 /,FPP/6HP2/P1 /,FRA/6HRHO2/R/,FRB/6HHO1   /,        000000
00120         1     FTT/6HP2/P1 /,FU1/6HU1  VE/,FU2/6HU2  VE/,FV21/6HV2(U1-/,        000000
00120         2     FV22/6HU2/M/S/,FV23/2HEC/                                        000000
00133          DOUBLE PRECISION G,GG,X                                               000000
00135          EQUIVALENCE (X(1),GG)                                                 000000
00135          LOGICAL EQL,INCDEQ,INCDFZ,SEQL,TP                                     000000
00135    C                                                                           000000
00136             LOGICAL ROYES                                                      000000
00136    C                                                                           000000
00137          REAL M1,MACH1,M2M1,MU12RT                                             000000
00137    C                                                                           000000
00140          NAMELIST /SHKINP/ GAMMA1,INCDEQ,INCDFZ,MACH1,U1              /SHKINP/ 000000
00140    C                                                                           000000
00141          IOF = 0                                                               000000
00142          TP=.TRUE.                                                             000000
00143          CPR1 = 0.                                                             000002
00144          DO 10 I=1,13                                                          000011
00147          MACH1(I)=0.                                                           000011
00150       10 U1(I) = 0.0                                                           000011
00152          GAMMA1 = 0.                                                           000013
00153          INCDEQ = .TRUE.                                                       000014
00154          INCDFZ = .TRUE.                                                       000016
00155          DO 18 I = 1,NREAC                                                     000022
00160       18 NAME(I,6)=IZERO                                                       000022
00162             CALL PAGIT                                                         000024
00163             CALL CHRSIZ(1)                                                     000026
00164             IF(RDYES('TYPE YES FOR PRESENT VALUES OF SHKINP NAMELIST',46))     000031
00164        1    WRITE(6,SHKINP)                                                    000031
00170             CALL CHRSIZ(4)                                                     000042
00171             CALL GOUT('TYPE NAMELIST  SHKINP HERE',21)                         000045
00172          READ (5,SHKINP)                                                       000051
00175          WRITE(JOUT,SHKINP)                                                    000055
00200          SEQL = INCDEQ                                                         000061
00201          IF (T(1) .LE. 0.0)  T(1) = RTEMP(1)                                   000063
00203          DO 20 I = 1,13                                                        000073
00206          IF (MACH1(I) .LE. 0.0 .AND. U1(I) .LE. 0.0)  GO TO 21                 000073
00210       20 NSK = I                                                               000107
```

```
00212      67*        21 IOF = IOF+1                                                          000114
00213      68*           OF = OXF(IOF)                                                        000117
00214      69*           CALL NEWOF                                                           000121
00215      70*           INCDEQ = SEQL                                                        000123
00216      71*        17 PP = P(1)                                                            000126
00217      72*           II = I(1)                                                            000127
00220      73*           IF (INCDEQ) GO TO 19                                                 000131
00220      74*     C  FROZEN                                                                  000131
00222      75*           DO 118 I = 1,13                                                      000136
00225      76*           DLVTP(I) = 1.0                                                       000136
00226      77*      118  DLVPT(I) = -1.0                                                      000137
00230      78*        19 DO 35  NPT=1,NSK                                                     000143
00233      79*           PPP(NPT) = P(NPT)                                                    000147
00234      80*           TTT(NPT) = T(NPT)                                                    000151
00235      81*           IF(NPT.EQ.1)  GO TO 14                                               000153
00237      82*           IF (PPP(NPT) .LE. 0.0)  PPP(NPT) = PPP(NPT-1)                        000156
00241      83*           IF (TTT(NPT) .LE. 0.0)  TTT(NPT) = TTT(NPT-1)                        000163
00243      84*           SSUM(NPT) = SSUM(NPT-1)                                              000170
00244      85*           HSUM(NPT) = HSUM(NPT-1)                                              000172
00245      86*           IF(           TTT(NPT).EQ.TT.AND.PPP(NPT).EQ.PP)  GO TO 15           000174
00247      87*        14 PP = PPP(NPT)                                                        000211
00250      88*           TT = TTT(NPT)                                                        000212
00251      89*           CALL HCALC                                                           000214
00252      90*           HSUM(NPT) = HSUBO                                                    000216
00253      91*       15  IF (CPR1 .GT. 0.0)  GAMMA1 = CPR1/(CPR1 - 1.0/AM1)                   000221
00255      92*           IF (GAMMA1 .GT. 0.0)  GO TO 30                                       000231
00257      93*           WRITE(JOUT,16)                                                       000234
00261      94*       16  FORMAT (//20X,34HMISSING GAMMA1 OR CP VALUE IN SHCK/)                000241
00262      95*           RETURN                                                               000241
00263      96*       30  A1 = SQRT(RBR*GAMMA1*TT/AM1)                                         000245
00264      97*           IF (U1(NPT) .LE. 0.0)  U1(NPT) = A1*MACH1(NPT)                       000255
00266      98*           IF (MACH1(NPT) .LE. 0.0)  MACH1(NPT) = U1(NPT)/A1                    000263
00270      99*           WM(NPT) = AM1                                                        000271
00271     100*           CPR(NPT) = CPR1                                                      000273
00272     101*       35  GAMMAS(NPT) = GAMMA1                                                 000275
00274     102*           EQL = .FALSE.                                                        000301
00274     103*     C  OUTPUT--1ST CONDITION                                                   000301
00275     104*           WRITE(JOUT,861)                                                      000302
00277     105*       861 FORMAT(1H1,43X,39HINCIDENT SHOCK WAVE PARAMETERS ASSUMING   )        000307
00300     106*           IF(.NOT.INCDEQ)  GO TO 44                                            000307
00302     107*                 WRITE(JOUT,862)                                                000311
00304     108*       862 FORMAT (1H ,51X,23HEQUILIBRIUM COMPOSITION  //)                      000316
00305     109*           GO TO 45                                                             000316
00306     110*        44             WRITE(JOUT,863)                                          000320
00310     111*       863 FORMAT (1H ,53X,18HFROZEN COMPOSITION //)                            000325
00311     112*        45 CALL OUT1                                                            000325
00312     113*           WRITE(JOUT,46)                                                       000326
00314     114*        46 FORMAT (16H INITIAL GAS (1) )                                        000336
00315     115*           FMT(3) = F13                                                         000336
00316     116*           FMT(4) = FOUR                                                        000340
00317     117*           WRITE(JOUT,FMT) FN,FB,(MACH1(J), J = 1,NPT)                          000342
00327     118*           FMT(4) = TWO                                                         000361
00330     119*           WRITE(JOUT,FMT) FU1,FVEL,(U1(J), J = 1,NPT)                          000363
00340     120*           CALL OUT2                                                            000401
00340     121*     C     BEGIN CALCULATIONS FOR 2ND CONDITION                                 000401
00341     122*           IF(INCDEQ)   EQL = .TRUE.                                            000403
```

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00343   123*        NPT = 1                                                          000407
00344   124*     47 GAMMA1 = GAMMAS(NPT)                                             000412
00345   125*        M1 = WM(NPT)                                                     000414
00346   126*        P1 = PPP(NPT)                                                    000416
00347   127*        T1 = TTT(NPT)                                                    000420
00350   128*        MS = HSUM(NPT)                                                   000422
00351   129*        P21 = (2.*GAMMA1*MACH1(NPT)**2-GAMMA1+1.)/(GAMMA1+1.)            000424
00352   130*        T21 = P21*(2./MACH1(NPT)**2+GAMMA1-1.)/(GAMMA1+1.)               000436
00353   131*        IF((T1*T21).GT.2000..AND. EQL) T21 = .7*T21 + 600./T1            000453
00355   132*        MU12RT = AM1*U1(NPT)**2/(RBR*T1)                                 000473
00356   133*        P21L=ALOG(P21)                                                   000503
00357   134*        T21L=ALOG(T21)                                                   000507
00360   135*        DO 100 I = 1,8                                                   000520
00363   136*        TT=T21*T1                                                        000520
00364   137*        PP=P21*P1                                                        000523
00365   138*        IF (.NOT.EQL) GO TO 40                                           000526
00367   139*        CALL EQLBRM                                                      000530
00370   140*        GO TO 50                                                         000532
00370   141*  C  FROZEN                                                              000532
00371   142*     40 TLN = ALOG (TT)                                                  000534
00372   143*        CALL MCALC                                                       000537
00373   144*        HSUM(NPT) = HSUBO                                                000542
00374   145*        CPR(NPT) = CPR1                                                  000544
00375   146*     50 RHO12 = M1*T21/(WM(NPT)*P21)                                     000543
00376   147*        GG=RHO12*MU12RT                                                  000556
00377   148*        G(1,1)=-GG*DLVPT(NPT)-P21                                        000564
00400   149*        G(1,2)=-GG*DLVTP(NPT)                                            000572
00401   150*        G(1,3)=P21-1.+MU12RT*(RHO12-1.)                                  000576
00402   151*        GG = (U1(NPT)*RHO12)**2/RBR                                      000605
00403   152*        G(2,1)=-GG*DLVPT(NPT)+TT*(DLVTP(NPT)-1.)/WM(NPT)                 000613
00404   153*        G(2,2)=-GG*DLVTP(NPT)-TT*CPR(NPT)                                000626
00405   154*        G(2,3) = HSUM(NPT) - MS - U1(NPT)**2*(1.0 - RHO12**2)/(2.0*RBR)  000636
00406   155*        X(3)=G(1,1)*G(2,2)-G(1,2)*G(2,1)                                 000652
00407   156*        X(1)=(G(1,3)*G(2,2)-G(2,3)*G(1,2))/X(3)                          000661
00410   157*        X(2)=(G(1,1)*G(2,3)-G(2,1)*G(1,3))/X(3)                          000671
00411   158*        AX = X(1)                                                        000701
00412   159*        AXX = X(2)                                                       000703
00413   160*        IF(AX.LT.0.) AX = -AX                                            000705
00415   161*        IF (AXX.LT.0.) AXX = -AXX                                        000712
00417   162*        IF (AXX.GT.AX)  AX = AXX                                         000717
00421   163*        IF(AX.LT..00005)  GO TO 150                                      000725
00423   164*        AX = AX/.4054652                                                 000731
00424   165*        IF(AX.LE.1.)  GO TO 75                                           000734
00426   166*        X(1) = X(1)/AX                                                   000737
00427   167*        X(2) = X(2)/AX                                                   000743
00430   168*     75 P21L=P21L+X(1)                                                   000750
00431   169*        T21L=T21L+X(2)                                                   000753
00432   170*        P21=EXP(P21L)                                                    000757
00433   171*    100 T21 = EXP(T21L)                                                  000763
00435   172*        WRITE(JOUT,125) U1(NPT)                                          000771
00440   173*    125 FORMAT(25H0DID NOT CONVERGE FOR U1=,F8.2,66H   ANSWERS PROBABLY NO  001001
00440   174*       1T RELIABLE, SOLUTION PROBABLY DOES NOT EXIST)                    001001
00441   175*    150 RRHO(NPT) = 1./RHO12                                             001001
00442   176*        M2M1(NPT) = WM(NPT)/AM1                                          001004
00443   177*        PCP(NPT) = P21                                                   001007
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ORIGINAL PAGE IS
OF POOR QUALITY

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00445    179*         IF (NPT .GE. IDEBUG .AND. IDEBUG .NE. 0) WRITE(JOUT,152) I,T21,P21        001013
00453    180*     152 FORMAT(10H0ITR NO.= ,I1,7X,7HT2/T1 =,F9.2,7X,7HP2/P1 =,F9.2 )             001036
00454    181*         UTWO(NPT) = U1(NPT)*RHO12                                                  001036
00455    182*         U1U2(NPT) = U1(NPT)-UTWO(NPT)                                              001042
00456    183*         IF(.NOT.EQL)  GO TO 161                                                    001044
00460    184*         DO 880 K=1,NS                                                              001047
00463    185*         IF(IUSE(K).LT.0)  GO TO 880                                                001057
00465    186*         IF(ENLN(K).GT.-87..AND.ENLN(K).LT.87.) EN(K,NPT) = EXP(ENLN(K))           001061
00467    187*     880 CONTINUE                                                                   001110
00471    188*         GO TO 431                                                                  001110
00471    189*   C  FROZEN                                                                        001110
00472    190*     161 PPP(NPT) = PP                                                              001112
00473    191*         TTT(NPT) = T                                                               001114
00474    192*         GAMMAS(NPT) = CPR(NPT)/(CPR(NPT) - 1.0/AM1)                               001116
00475    193*     431 ISV = 0                                                                    001125
00476    194*         IF(NPT.LT.NSK)  ISV=NPT                                                    001126
00500    195*         IF(NPT.EQ.1)  ISV=-1                                                       001133
00502    196*         NPT = NPT+1                                                                001140
00503    197*         IF(EQL)  CALL SAVE                                                         001146
00505    198*         IF(NPT.LE.NSK)  GO TO 47                                                   001147
00507    199*         NPT = NSK                                                                  001153
00507    200*   C  OUTPUT--2ND CONDITION                                                         001153
00510    201*         WRITE(JOUT,58)                                                             001156
00512    202*      58 FORMAT (16H0SHOCKED GAS (2) )                                              001162
00513    203*         FMT(4) = TWO                                                               001162
00514    204*         WRITE(JOUT,FMT) FU2,FVEL,(UTWO(J),J = 1,NPT)                              001164
00524    205*         CALL OUT2                                                                  001204
00525    206*         WRITE(JOUT,68)                                                             001206
00527    207*      68 FORMAT (26H0INCIDENT SHOCK PARAMETERS  )                                   001216
00530    208*         FMT(4) = THREE                                                             001216
00531    209*         WRITE(JOUT,FMT) FPP,FB,FB,(PCP(J), J = 1,NPT)                             001220
00542    210*         WRITE(JOUT,FMT) FTT,FB,FB,(T2T1(J), J = 1,NPT)                            001235
00553    211*         FMT(4) = FOUR                                                              001252
00554    212*         WRITE(JOUT,FMT) FMM,FB,FB,(M2M1(J), J = 1,NPT)                            001254
00565    213*         WRITE(JOUT,FMT) FRA,FRB,FB,(RRHO(J), J = 1,NPT)                           001271
00576    214*         FMT(4) = TWO                                                               001304
00577    215*         WRITE(JOUT,FMT) FV21,FV22,FV23,(U1U2(J), J = 1,NPT)                       001310
00610    216*         CALL OUT3                                                                  001325
00611    217*         INCDEQ = .FALSE.                                                           001327
00612    218*         IF(INCDFZ.AND.EQL)  GO TO 17                                               001330
00614    219*         IF(IOF.LT.NOF)  GO TO 21                                                   001333
00616    220*         TP = .FALSE.                                                               001341
00617    221*         DO 999 K = 1,NREAC                                                         001345
00622    222*     999 RTEMP(K) = T(1)                                                            001345
00624    223*         RETURN                                                                     001347
00625    224*         END                                                                        001400

      END OF COMPILATION:         NO  DIAGNOSTICS.


@HDG,P      THERMP
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THERMP                                                                              DATE 101580        PAGE     1

@FOR,S    THERMP,THERMP
H$A  E3 -10/15/80-13:07:55 (19,)

   SUBROUTINE THERMP     ENTRY POINT 000427

   STORAGE USED: CODE(1) 000437; DATA(0) 000117; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   CONSTS  000006
    0004   POINTS  000335
    0005   MISC    001701
    0006   INDX    000041
    0007   OUPT    000073
    0010   CCC     000003
    0011   CFUEL   000002

   EXTERNAL REFERENCES (BLOCK, NAME)

    0012   NEWOF
    0013   EQLBRM
    0014   MOVABS
    0015   HOLDIT
    0016   PAGIT
    0017   GOUT
    0020   OUT1
    0021   OUT2
    0022   OUT3
    0023   OUT4
    0024   SAVE
    0025   NWDUS
    0026   NIO2$
    0027   NIO1$
    0030   NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000   000021 10F       0000   000025 11F       0000   000033 12F       0001   000022 1256      0001   000044 1326
    0000   000041 20F       0000   000045 21F       0000   000054 22F       0001   000234 2256      0001   000261 2416
    0000   000006 5F        0001   000061 800L      0001   000111 860L      0001   000162 861L      0001   000207 862L
    0000   000062 863F      0001   000265 864L      0000   000070 858F      0001   000354 870L      0001   000463 871L
    0001   000276 902L      0001   000006 95L       0005   000640 AM        0005   000705 AM1       0005   001135 ANUM
    0003   000000 ATMN      0005   000004 ATOM      0005   000514 BO        0005   000545 BOP       0006   000036 CALCH
    0011 R 000000 CF        0006   000001 CONVG     0004   000032 CPR       0005   000706 CPR1      0005   000634 CPSUM
    0005   000654 DATA      0010   000002 DEMAND    0005   001560 DENS      0004   000064 DLVPT     0004   000047 DLVTP
    0005   001700 ENLSAV    0005   000000 ENN       0005   001676 ENNL      0005   001677 ENSAVE    0005   001414 ENTH
    0005   000636 EQRAT     0007   000002 FA        0007   000063 FAP       0005   001445 FA2       0007 R 000005 FB
    0007   000006 FC        0007   000007 FCP       0007   000012 FCST      0007   000014 FCV       0007   000015 FG
    0007   000017 FGE       0007   000020 FGV       0007   000021 FH        0007   000023 FI        0007   000025 FIV
    0007   000027 FM        0007 R 000031 FMT       0007   000050 FN        0007   000052 FOUR      0005   001527 FOX
    0007   000053 FP        0007   000054 S         0007   000056 FSV       0007   000057 FT        0007   000061 FTR
    0000 R 000000 FUA       0000 R 000001 FUB       0007   000063 FV        0007   000065 FVEL      0007   000001 F13
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0007     000000 F9X       0004     000101 GAMMAS    0003     000001 GMZT      0010     000000 GRAPH     0011     000001 HHVV
0006 L   000003 HP        0005     000442 HPP       0005 R   000637 HSUBO     0004     000000 HSUM      0000 I   000003 I
0006     000030 IC        0006 I   000000 IDEBUG    0006     000015 IMAT      0000     000100 INJP$     0000 I   000002 IOF
0006     000023 IONS      0006 I   000021 IP        0006     000037 IOSAVE    0006     000016 IO1       0006 I   000005 ISV
0006 I   000034 IT        0006     000026 JLIO      0010 I   000001 JOUT      0006     000025 JSOL      0006     000031 JS1
0006     000014 KMAT      0005     000463 LLMT      0006     000040 LSAVE     0006     000006 MOLES     0004     000707 NAME
0006     000024 NC        0006     000022 NEWR      0006     000035 NFZ       0006     000012 NLM       0006 I   000017 NOF
0006     000020 NOMIT     0006 I   000007 NP        0006 I   000011 NPT       0006     000027 NREAC     0006     000013 NS
0006 I   000010 NT        0005 R   000635 OF        0007 R   000067 ONE       0005 R   001644 OXF       0004 R   000116 P
0003     000002 PATM      0005     001363 PECUT     0005 R   000633 PP        0004     000217 PPP       0003 R   000003 RBAR
0003     000004 RBR       0005     000644 RM        0005     001611 RMOP      0005     001612 RMW       0005     001476 RTEMP
0003     000005 RYR       0006     000033 SHOCK     0004     000251 SONVEL    0006 L   000004 SP        0004     000015 SSUM
0005     000001 SUMN      0005     000003 SO        0004 R   000150 T         0005     000632 THIGH     0007     000070 THREE
0005     001643 TLN       0005     000630 TLOW      0005     000627 TM        0005     000631 TMID      0004     000320 TOTN
0006 L   000002 TP        0005 R   000702 TT        0004     000266 TTT       0007 R   000071 TWO       0004 R   000202 V
0004 R   000303 VLM       0005     000646 VMIN      0006 L   000032 VOL       0005     000650 VPLS      0004     000234 WM
0005     000652 WP        0007     000072 ZERO
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00101      1*           SUBROUTINE THERMP                                                              000000
00101      2*     C                                                                        MOLI0001    000000
00103      3*           COMMON /CONSIS/ ATMN,GMEI,P,TM,RBAR,RBR,RYR                        /CONSIS/    000000
00104      4*           COMMON/POINTS,HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                    000000
00104      5*          1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)               000000
00104      6*          2 ,VLM(13),TOTN(13)                                                             000000
00105      7*           COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                      000000
00105      8*          1                BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                000000
00105      9*          2                HSUBO,AM(2),HPP(2),RM(2),VMIN(2),VPLS(2),WP(2),    /MISC/      000000
00105     10*          3                DATA(25),AM3,CPR1,NAME(25,6),ANUM(25,6),PECUT(25),             000000
00105     11*          4                ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,              000000
00105     12*          5                RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                         000000
00106     13*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/      000000
00106     14*          1                KMAT,IMAT,IO1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIO,   /INDX/      000000
00106     15*          2                NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCM,IOSAVE,LSAVE    /INDX/      000000
00107     16*           COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),    /OUPT/      000000
00107     17*          1                FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/    000000
00107     18*          2                FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,  /OUPT/     000000
00107     19*          3                TWO,ZERO                                           /OUPT/      000000
00107     20*     C                                                                                    000000
00110     21*             COMMON /CCC/ GRAPH,JOUT,DEMAND                                               000000
00110     22*     C                                                                                    000000
00111     23*           COMMON /CFUEL/CF,HHVV                                                          000000
00112     24*           DATA FUA/6HU CAL//,FUB/6HGRAM  /                                               000000
00115     25*           LOGICAL HP,SP,TP,VOL                                                           000000
00115     26*     C                                                                                    000000
00116     27*           IF (T(1) .LE. 0.0)  T(1) = 3800.0                                              000000
00120     28*           IOF = 0                                                                        000004
00121     29*        95 IOF = IOF+1                                                                    000006
00122     30*           OF = OXF(IOF)                                                                  000011
00123     31*           CALL NEWOF                                                                     000013
00123     32*     C     SET ASSIGNED P OR VOLUME                                                       000013
00124     33*           DO 871 IP = 1,NP                                                               000015
00127     34*           PP = P(IP)                                                                     000035
00130     35*           VLM(NPT) = P(IP)                                                               000037
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00130     36*    C      SET ASSIGNED T                                                  MOLI0016    000037
00131     37*           DO 871 IT = 1,NT                                                            000044
00134     38*           TT = T(IT)                                                      MOLI0019    000044
00135     39*           CALL EQLBRM                                                     MOLI0025    000046
00136     40*           IF (TT .GT. 0.0)  GO TO 800                                                 000050
00140     41*           IF (NPT .EQ. 0)  RETURN                                                     000053
00142     42*       800 ISV = 0                                                                     000061
00143     43*           IF (IP .EQ. NP .AND. IT .EQ. NT .OR. TT .LE. 0.0)  GO TO 860                000061
00145     44*           ISV = NPT                                                                   000104
00146     45*           IF(NPT.NE.13)  GO TO 870                                        MOLI0030    000106
00150     46*       860 CONTINUE                                                                    000111
00151     47*           CALL MOVARS(S00,S0)                                                         000111
00152     48*           CALL MOLDIT                                                                 000114
00153     49*           CALL PAGIT                                                                  000116
00154     50*           CALL GOUT(' ',1)                                                            000120
00155     51*           WRITE (JOUT,5)                                                              000124
00157     52*         5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNEDMOLI0032  000131
00157     53*          1)                                                                           000131
00160     54*           IF(.NOT.VOL)  GO TO 861                                                     000131
00162     55*           IF (HP)  WRITE(JOUT,10)                                                     000133
00165     56*        10 FORMAT(1H0,62X,7H VOLUME /)                                                 000142
00166     57*           IF (TP)  WRITE(JOUT,11)                                                     000142
00171     58*        11 FORMAT(1H0,53X,22HTEMPERATURE AND VOLUME/)                                  000151
00172     59*           IF (SP)  WRITE(JOUT,12)                                                     000151
00175     60*        12 FORMAT(1H0,56X,18HENTROPY AND VOLUME/)                                      000160
00176     61*           GO TO 862                                                                   000160
00177     62*       861 IF(HP)  WRITE(JOUT,20)                                                      000162
00202     63*        20 FORMAT(1H0,62X,10H PRESSURES  /)                                            000170
00203     64*           IF(TP)  WRITE(JOUT,21)                                                      000170
00206     65*        21 FORMAT(1H0,53X,24HTEMPERATURE AND PRESSURE/)                                000177
00207     66*           IF(SP)  WRITE(JOUT,22)                                                      000177
00212     67*        22 FORMAT(1H0,55X,20HENTROPY AND PRESSURE/)                                    000207
00213     68*       862 CALL OUT1                                                                   000207
00214     69*           WRITE(JOUT,863)                                                             000210
00216     70*       863 FORMAT (25H0THERMODYNAMIC PROPERTIES//)                                     000223
00217     71*           IF(.NOT.VOL)  GO TO 869                                                     000223
00221     72*           FMT(3) = ONE                                                                000225
00222     73*           IF (.NOT. HP)  GO TO 864                                                    000227
00224     74*           DO 63 I=1,NPT                                                               000234
00227     75*           FMT(I+2) = TWO                                                              000234
00230     76*           IF (I .EQ. 13)  FMT(15) = 5HF9.2)                                           000236
00232     77*        63 V(I) = RBAR*HSUB0                                                           000243
00234     78*           WRITE(JOUT,FMT) FUA,FUB,FD,(V(I), I = 1,NPT)                                000247
00245     79*       864 CALL OUT2                                                                   000265
00246     80*           CALL OUT3                                                                   000266
00247     81*           IF (CF-1.0) ,902,                                                           000270
00252     82*       900 CALL OUT4                                                                   000273
00253     83*       902 CONTINUE                                                                    000276
00254     84*           CALL MOVARS(S00,S0)                                                         000276
00255     85*           CALL MOLDIT                                                                 000301
00256     86*           CALL PAGIT                                                                  000303
00257     87*           IF (ISV .EQ. 0 .AND. IOF .EQ. NOF)  RETURN                                  000305
00261     88*           IF(IDEBUG.GT.13)  IDEBUG=IDEBUG-13                                          000322
00263     89*           WRITE(JOUT,868)                                                             000331
00265     90*       868 FORMAT(1H1)                                                                 000336
00266     91*           IF(NT.EQ.1.AND.NP.EQ.1)  GO TO 95                                           000336
```

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```
00270      92*         NPT = 0                                          000352
00271      93*     870 NPT = NPT + 1                           NOLI0037     000354
00272      94*         IF(.NOT.TP)  T(1)=TT                                 000356
00274      95*         IF (IP.EQ.1.AND.IT.EQ.1)  ISV=-ISV            12-22  000362
00276      96*         IF(NT.EQ.1)  GO TO 871                        12-22  000373
00300      97*         IF(IT.EQ.NT)  ISV=0                                  000376
00302      98*     871 CALL SAVE                                            000403
00305      99*         GO TO 95                                             000410
00306     100*         END                                     NOLI0045     000436

     END OF COMPILATION:          NO DIAGNOSTICS.

@HDG,P       VARFMT
```

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```
VARFMT                                                                                   DATE 101580        PAGE     1

@FOR,S    VARFMT,VARFMT
HSA  E3 -10/15/80-13:07:58 (7,)

   SUBROUTINE VARFMT    ENTRY POINT 000115

   STORAGE USED: CODE(1) 000124; DATA(0) 000023; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   OUPT   000073

   EXTERNAL REFERENCES (BLOCK, NAME)

    0004   NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001      000006 1146         0001     000046 40L         0001      000100 45L         0003      000002 FA          0003      000003 FAP
    0003      000005 FB           0003     000006 FC          0003      000007 FCP         0003      000012 FCST        0003      000014 FCV
    0000 R    000000 FFOUR        0003     000015 FG          0003      000017 FGE         0003      000020 FGV         0003      000021 FH
    0003      000023 FI           0003     000025 FIV         0003      000027 FM          0003 R    000031 FMT         0003      000050 FN
    0000 R    000001 FONE         0003 R   000052 FOUR        0003      000053 FP          0003      000054 FS          0003      000056 FSV
    0003      000057 FT           0000 R   000002 FTHREE      0003      000061 FTK         0000 R    000003 FTWO        0003      000063 FV
    0003      000065 FVEL         0000 R   000004 FZERO       0003      000001 F13         0003      000000 F9X         0000 I    000005 I
    0000      000012 INJPS        0003 R   000067 ONE         0003 R    000070 THREE       0003 R    000071 TWO         0003 R    000072 ZERO


 00101      1*            SUBROUTINE VARFMT(V,NPT)                                                  000006
 00101      2*      C                                                                               000006
 00103      3*            COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),    /OUPT/  000006
 00103      4*           1         FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/      000006
 00103      5*           2         FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/      000006
 00103      6*           3         TWO,ZERO                                             /OUPT/      000006
 00103      7*      C                                                                               000006
 00104      8*            DATA FFOUR/5HF9.4)/,FONE/5HF9.1)/,FTHREE/5HF9.3)/,FTWO/5HF9.2)/,          000006
 00104      9*           1   FZERO/5HF9.0)/                                                         000006
 00112     10*            DIMENSION V(13)                                                           000006
 00112     11*      C                                                                               000006
 00113     12*            DO 45 I = 1,NPT                                                           000006
 00116     13*            IF (I .GE. 13)  GO TO 40                                                  000006
 00120     14*            FMT(I+2) = FOUR                                                           000012
 00121     15*            IF (V(I) .GE. 10.0)  FMT(I+2) = THREE                                     000014
 00123     16*            IF (V(I) .GE. 100.0)  FMT(I+2) = TWO                                      000022
 00125     17*            IF (V(I) .GE. 1.0E4)  FMT(I+2) = ONE                                      000030
 00127     18*            IF (V(I) .GE. 1.0E6)  FMT(I+2) = ZERO                                     000036
 00131     19*            GO TO 45                                                                  000044
 00132     20*        40  FMT(15) = FFOUR                                                           000046
 00133     21*            IF (V(I) .GE. 10.0)  FMT(15) = FTHREE                                     000047
 00135     22*            IF (V(I) .GE. 100.0)  FMT(15) = FTWO                                      000055
 00137     23*            IF (V(I) .GE. 1.0E4)  FMT(15) = FONE                                      000063
```

```
                                                                           DATE 101580       PAGE    2
     VARFMT
                                                                              000071
  00141      24*           IF (V(I) .GE. 1.0E6)  FMT(15) = FZERO              000102
  00143      25*        45 CONTINUE                                           000102
  00145      26*           RETURN                                             000123
  00146      27*           END

         END OF COMPILATION:         NO  DIAGNOSTICS.


  @END
  @END IGNORED - IN CONTROL MODE

  @FIN
```

```
RUNID, LEWIST   ACCT: 1HPA01R5002:   PROJECT: SEVIGWBIN2D8
     LOAD 15753 11/0 PUR -1 LEWIST
TIME:      SUPS: 00:02:51.912       CBSUPS:  057007923
            CPU:  00:00:38.729      I/O:  00:01:29.681
          CC/ER: 00:00:43.5C1       WAIT: 00:00:00.065
IMAGES  READ:   61        PAGES:  118
START:    13:04:46 OCT 15,1980     FIN:  13:08:01 OCT 15,1980
THE 1108 (HOST2) WILL BE POWERED OFF NO LATER THAN NOV 15 1980
```

```
12345678   2345678901234567890123456789012345678901234567890123456789   901234567890123456789012345678901234567890123456789 0*** . NO. 07

* * * * * * UNIVAC 1100 TIME/SHARING EXEC  ACCOUNT NUMBER * 1HPA01R50021 VER. EN 33R3HOST2 SITE *  HOST 2  * * * * * *

123456   012345678901234567890123456789012345678901234567890123
```

APPENDIX C

SOURCE LISTING OF PROGRAM ELEMENTS WITHOUT MODIFICATIONS

This is a printout of the Lewis Chemical Equilibrium Program without the modifications necessary for coal gasification data. There have been intermediate changes, principally to make the program an interactive one.

```
        JJ      NN        NN      00000000         999999           11                44  44
        JJ      NNN       NN     0000000000      9999999999        111               44   44
        JJ      NNNN      NN    00        00    99        99      1111              44    44
        JJ      NNNNN     NN    00        00    99        99        11             44     44
        JJ      NN NNN    NN    00        00    99        99        11            44      44
        JJ      NN  NNN   NN    00        00     99999999999        11           44444444444
        JJ      NN   NNN  NN    00        00      9999999 99        11          444444444444
        JJ      NN    NNN NN    00        00              99        11                    44
        JJ      NN     NNNNN    00        00              99        11                    44
JJ      JJ      NN      NNNN    00        00    99        99        11                    44
 JJJJJJJJJ      NN       NNN     0000000000      9999999999       111111                  44
  JJJJJJJ       NN        NN      00000000         999999         111111                  44

NN        NN      OOOOOOOO      LL                AAAAAAAA      NN        NN    DDDDDDDDDD
NNN       NN     OOOOOOOOOO     LL               AAAAAAAAAA     NNN       NN    DDDDDDDDDDD
NNNN      NN    OO        OO    LL              AA        AA    NNNN      NN    DD        DD
NNNNN     NN    OO        OO    LL              AA        AA    NNNNN     NN    DD        DD
NN NNN    NN    OO        OO    LL              AA        AA    NN NNN    NN    DD        DD
NN  NNN   NN    OO        OO    LL              AAAAAAAAAAAA    NN  NNN   NN    DD        DD
NN   NNN  NN    OO        OO    LL              AAAAAAAAAAAA    NN   NNN  NN    DD        DD
NN    NNN NN    OO        OO    LL              AA        AA    NN    NNN NN    DD        DD
NN     NNNNN    OO        OO    LL              AA        AA    NN     NNNNN    DD        DD
NN      NNNN    OO        OO    LL              AA        AA    NN      NNNN    DD        DD
NN       NNN     OOOOOOOOOO     LLLLLLLLLLLL    AA        AA    NN       NNN    DDDDDDDDDDD
NN        NN      OOOOOOOO      LLLLLLLLLLLL    AA        AA    NN        NN    DDDDDDDDDD

BBBBBBBBBB        IIIIII        NN        NN       222222           0000          888888
BBBBBBBBBBB       IIIIII        NNN       NN     2222222222       00000000       88888888
BB        BB        II          NNNN      NN    222      222     000    000     88      88
BB        BB        II          NNNNN     NN    22       222    000    0000     88      88
BB        BB        II          NN NNN    NN            222     00    00  00     88    88
BBBBBBBBBB          II          NN  NNN   NN           222      00   00   00      888888
BBBBBBBBBB          II          NN   NNN  NN          222       00  00    00     8888888888
BB        BB        II          NN    NNN NN         222        00 00     00    888      888
BB        BB        II          NN     NNNNN       222          0000     000    88        88
BB        BB        II          NN      NNNN      222            000    000     888      888
BBBBBBBBBBB       IIIIII        NN       NNN    222222222222      00000000       8888888888
BBBBBBBBBB        IIIIII        NN        NN    222222222222        0000          88888888

* * * * * * UNIVAC 1100 TIME/SHARING EXEC  ACCOUNT NUMBER * IHPDU13K0000 VER. CR 33R3H0S11 SITE * HOST 1  * * * * * *

  RUNID * JN0914        USER ID *                  PART NUMBER * 01      INPUT DEVICE * DTRDU4        OUTPUT DEVICE * PR2

    FILE NAME * PRT                  CREATED AT:   17:37:49 OCT 25,1979           PRINTED AT:   17:43:59 OCT 25,1979
```

① SPECIES DIMENSIONS CHANGED TO 150.

② MAIN PROGRAM MODIFIED TO PREVENT PAGE RESET

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```
@FOR,S LEWIS.BLOCK1,LEWIS.BLOCKB
FOR 13 -10/25/79-17:37:50 (0,)

   BLOCK DATA

   STORAGE USED: CODE(1) 000000; DATA(0) 000000; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSTS 000006
    0004    MOLCON 000010
    0005    MISC   001264
    0006    OUPT   000073

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0005   000570 AM        0005   000624 AM1       0005   000741 ANUM      0005 R 000004 ATAM      0005 R 000235 ATEM
    0003 R 000000 ATMN      0005   000004 ATOM      0005   000502 BO        0005   000521 BUP       0005   000625 CPR1
    0005   000564 CPSUM     0005   000604 DATA      0005   001107 DENS      0004 R 000000 END       0005   001263 ENLSAV
    0005   000000 ENN       0005   001261 ENNL      0005   001262 ENSAVE    0005   001073 ENMF      0005   000566 EQRAT
    0006 R 000002 FA        0006 R 000003 FAP       0005   001112 FAZ       0006 R 000005 FB        0006 R 000004 FC
    0006 R 000007 FCP       0006 R 000012 FCST      0006 R 000014 FCV       0006 R 000015 FG        0006 R 000017 FGE
    0006 R 000020 FGV       0006 R 000021 FH        0006 R 000023 FI        0006 R 000025 FIV       0006 R 000027 FM
    0006 R 000031 FMT       0006 R 000050 FN        0006 R 000052 FOUR      0005   001150 FOX       0006 R 000053 FP
    0006 R 000054 FS        0006 R 000056 FSV       0006 R 000057 FT        0006 R 000061 FTK       0006 R 000063 FV
    0006 R 000065 FVEL      0006 R 000001 F13       0006 R 000000 F9X       0004 R 000001 GAS       0003 R 000001 GMET
    0005   000572 HPP       0005   000567 HSUBO     0004 I 000002 IE        0004 I 000003 IZERO     0004 I 000004 LANN
    0005   000463 LLMT      0004 I 000005 MOL       0005   000626 NAME      0005   000565 OF        0006 R 000067 ONE
    0004 R 000006 OX        0005   001227 OXF       0003 R 000002 PATM      0005   001054 PECWT     0005   000563 PP
    0003 R 000003 RBAR      0003 R 000004 RBR       0005   000574 RH        0005   001206 RHOP      0005   001207 RMW
    0005   001131 RTEMP     0003 R 000005 RVR       0005   000001 SUMN      0005   000003 SO        0005   000562 THIGH
    0006 R 000070 THREE     0005   001226 TLN       0005   000560 TLOW      0005   000557 TM        0005   000561 TMID
    0005   000002 TT        0006 R 000071 TWO       0005   000576 VMIN      0005   000600 VPLS      0005   000602 WP
    0004 R 000007 ZERO      0006 R 000072 ZEROF


00101       1*          BLOCK DATA                                                                ATM000001    000000
00101       2*     C                                                                                           000000
00102       3*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                               /CONSTS/     000000
00103       4*          COMMON /MOLCON/ END,GAS,IE,IZERO,LANN,MOL,OX,ZERO                         /MOLCON/     000000
00104       5*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),                 /MISC/       000000
00104       6*    1                   BUP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,             /MISC/       000000
00104       7*    2                   HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),             /MISC/       000000
00104       8*    3                   DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),          /MISC/       000000
00104       9*    4                   RMW(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,            /MISC/       000000
00104      10*    5                   AMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                      /MISC/       000000
00105      11*          COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),           /OUPT/       000000
00105      12*    1                   FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR,        /OUPT/       000000
00105      13*    2                   FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,          /OUPT/       000000
00105      14*    3                   TWO,ZEROF                                                   /OUPT/       000000
00105      15*     C                                                                                           000000
00106      16*          DIMENSION ATAM(3,51),ATEM(3,50)                                                        000000
00107      17*          EQUIVALENCE (ATOM(1,1),ATAM),(ATOM(1,52),ATEM)                                         000000
```

```
00107     C                                                                          000000
00107     C   ATOMIC SYMBOLS, WEIGHTS, AND VALENCES                                  000000
00110          DATA ATAM/2HH ,1.00797,1.0,2HHE,4.0026,0.0,2HLI,6.939,1.0,2HBE,        000000
00110         1 9.0122,2.0,2HB ,10.811,3.0,2HC ,12.01115,4.0,2HN ,14.0067,0.0,        000000
00110         2 2HO ,15.9994,-2.0,2HF ,18.9984,-1.0,2HNE,20.183,0.0,2HNA,22.9898,     000000
00110         3 1.0,2HMG,24.312,2.0,2HAL,26.9815,3.0,2HSI,28.086,4.0,2HP ,30.9738     000000
00110         4,5.0,2HS ,32.064,4.0,2HCL,35.453,-1.0,2HAR,39.948,0.0,2HK ,39.102,     000000
00110         5 1.0,2HCA,40.080,2.0,2HSC,44.956,3.0,2HTI,47.90,4.0,2HV ,50.942,       000000
00110         6 5.0,2HCR,51.996,3.0,2HMN,54.9380,2.0,2HFE,55.847,3.0,2HCO,58.9332     000000
00110         7,2.0,2HNI,58.710,2.0,2HCU,63.540,2.0,2HZN,65.370,2.0,2HGA,69.720,      000000
00110         8 3.0,2HGE,72.590,4.0,2HAS,74.9216,3.0,2HSE,78.960,4.0,2HBR,79.909,     000000
00110         9 -1.0,2HKR,83.80,0.0,2HRB,85.47,1.0,2HSR,87.620,2.0,2HY ,88.905,       000000
00110         A 3.0,2HZR,91.220,4.0,2HNB,92.906,5.0,2HMO,95.94,6.0,2HTC,99.0,7.0,     000000
00110         B 2HRU,101.070,3.0,2HRH,102.905,3.0,2HPD,106.40,2.0,2HAG,107.870,       000000
00110         C 1.0,2HCD,112.40,2.0,2HIN,114.820,3.0,2HSN,118.690,4.0,2HSB,           000000
00110         D 121.750,3.0/                                                          000000
00112          DATA ATEM/2HTE,127.60,4.0,2HI ,126.9044,-1.0,2HXE,131.30,0.0,2HCS,     000000
00112         1 132.905,1.0,2HBA,137.340,2.0,2HLA,138.910,3.0,2HCE,140.120,3.0,       000000
00112         2 2HPR,140.907,3.0,2HND,144.240,3.0,2HPM,145.0,3.0,2HSM,150.350,3.0     000000
00112         3,2HEU,151.960,3.0,2HGD,157.250,3.0,2HTB,158.924,3.0,2HDY,162.50,       000000
00112         4 3.0,2HHO,164.930,3.0,2HER,167.260,3.0,2HTM,168.934,3.0,2HYB,          000000
00112         5 173.040,3.0,2HLU,174.997,3.0,2HHF,178.490,4.0,2HTA,180.948,5.0,       000000
00112         6 2HW ,183.850,6.0,2HRE,186.20,7.0,2HOS,190.20,4.0,2HIR,192.20,4.0,     000000
00112         7 2HPT,195.090,4.0,2HAU,196.967,3.0,2HHG,200.590,2.0,2HTL,204.370,      000000
00112         8 1.0,2HPB,207.190,2.0,2HBI,208.980,3.0,2HPO,210.0,2.0,2HAT,210.0,      000000
00112         9 0.0,2HRN,222.0,0.0,2HFR,223.0,1.0,2HRA,226.0,2.0,2HAC,227.0,3.0,      000000
00112         A 2HTH,232.038,4.0,2HPA,231.0,5.0,2HU ,238.030,6.0,2HNP,237.0,5.0,      000000
00112         B 2HPU,242.0,4.0,2HAM,243.0,3.0,2HCM,247.0,3.0,2HBK,249.0,3.0,2HCF,     000000
00112         C 251.0,3.0,2HES,254.0,0.0,2HFM,253.0,0.0,2HD ,2.014102,1.0/            000000
00112     C      INFORMATION USED IN VARIABLE OUTPUT FORMAT                           000000
00114          DATA F9X/3H9X,/,F13/2H13/,FA/6HAE/AT /,FB/6H      /,FC/6HCF     /,  /OUPT/  000000
00114         1      FCV/6HCF VAC/,F6/12HGAMMA (S)   /,FI/12HISP SECONDS /,        /OUPT/  000000
00114         2      FIV/12HIVAC SECONDS/,FM/12HM MOL WEIGHT/,FMT/6H(1H ,2,        /OUPT/  000000
00114         3      6HA6,A2,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,     /OUPT/  000000
00114         4      5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1)/,     /OUPT/  000000
00114         5      FN/12HMACH NUMBER /,FOUR/5HF9.4,/,FP/6HPC/P  /,               /OUPT/  000000
00114         6      FT/12H(DLV/DLP) T /,FV/12H(DLV/DLT) P /,ONE/5HF9.1,/,         /OUPT/  000000
00114         7      THREE/5HF9.3,/,TWO/5HF9.2,/,ZEROF/5HF9.0,/,FAP/12HPRESS N/M**            000000
00114         82/,FCP/12HCP CAL/(G)(K,2H) /,FCST/12HCSTAR M/SEC /,FGE/6H(EFF) /,               000000
00114         9 FGV/6HGAS VL/,FH/12HENTH CAL/G  /,FS/12HS CAL/(G)(K)/,FSV/6HSON V               000000
00114         AE/,FTR/12HTEMP DEG. K /,FVEL/6HL M/SE,2HC /                                     000000
00123          DATA END/3HEND/,GAS/1HG/,IE/1HE/,IZERO/2H00/,LANR/2H  /,MOL/1HM/                000000
00123         1 ,OX/1HO/,ZERO/1H0/,ATMM/101325.0/,RVR/82.0554997/                              000000
00123         3 ,GMLT/9.80665D/,PATM/14.696006D/,RBAR/1.987165D/,RBR/8314.29036D/              000000
00142          END                                                              ATM00060      000000
END FCN
```

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```
@FOR,S LEWIS.CPHS,LEWIS.CPHS
H,A  L: -10/25/79-17:37:57 (9,)


   SUBROUTINE CPHS      ENTRY POINT 000567


   STORAGE USED: CODE(1) 000603; DATA(0) 000160; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   SPECES 012120
    0004   MISC   001264
    0005   INDX   000041
    0006   COMTH  001201
    0007   CCC    000003


   EXTERNAL REFERENCES (BLOCK, NAME)

    0010   NWDU$
    0011   NIO2$
    0012   ALOG
    0013   NIO1$
    0014   NERR3$


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   000031 10L       0001   000207 171G      0001   000217 174G      0001   000043 20L       0001   000351 221G
    0001   000462 254G      0001   000065 30L       0001   000067 31L       0001   000157 32L       0000   000041 3333F
    0001   000164 40L       0001   000176 60L       0001   000230 70L       0001   000233 80L       0001   000412 87L
    0004   000060 6AF       0001   000472 69L       0001   000531 90L       0000   000103 904F      0003   006034 A
    0004   000570 AM        0004   000624 AM1       0004   000741 ANUM      0004   000004 ATOM      0004   000502 BO
    0004   000521 BOP       0005   000036 CALCH     0003 R 000000 COEF      0005   000001 CONVG     0006 R 000361 CPL
    0004   000625 CPHI      0004 R 000564 CPSUM     0000 R 000040 CPUSED    0000 R 000035 CPX       0000 R 000007 CPXX
    0004   000604 DATA      0003   005670 DELN      0007   000002 DEMAND    0004   001167 DENS      0003 R 002734 EN
    0003   005360 ENLN      0004   001263 ENLSAV    0004   000000 ENN       0004   001261 ENNL      0004   001262 ENSAVE
    0004   001073 ENTH      0004   000566 EQRAT     0004   001112 FAZ       0004   001150 FOX       0007   000000 GRAPH
    0006 R 000551 HL        0005   000003 HF        0004   000572 HPP       0004   000567 HSUBO     0000 R 000034 HX
    0000 R 000013 HXX       0003 R 005524 HO        0000 I 000037 I         0005   000030 IC        0005   000000 IDEBUG
    0000 I 000001 IER       0000 I 000023 IEXTND    0006 I 001131 ILSP      0005   000015 IMAT      0000 I 000002 IMSG
    0000   000132 INJF$     0005   000023 IONS      0005   000021 IP        0005   000037 IQSAVE    0005   000016 IQ1
    0005   000035 ISV       0005   000034 IT        0003 I 011444 IUSE      0000 I 000026 IX        0005 I 000031 J
    0005   000026 JCIQ      0007 I 000001 JOUT      0005   000025 JSOL      0000 I 000024 K         0000 I 000025 KK
    0005   000014 KMAT      0000 I 000027 KX        0004   000463 LLMT      0005   000040 LSAVE     0000 I 000036 M
    0005   000006 MOLES     0004   000626 NAME      0005   000024 NC        0005   000022 NEWR      0005   000035 NFZ
    0005   000012 NLM       0006 I 000000 NLTSP     0005   000017 NOF       0005   000020 NOMIT     0005   000007 NP
    0000 I 000011 NPI       0005   000027 NREAC     0005 I 000013 NS        0000 I 000000 NSPP1     0005   000010 NT
    0000 I 000030 NTOP      0004   000565 OF        0004   001227 OXF       0004   001054 PECWT     0004   000563 PP
    0004   000474 RH        0004   001206 RHOP      0004   001207 RHW       0004   001131 RTEMP     0003 R 002570 S
    0005   000033 SHOCK     0006 R 000741 SL        0003   011754 SLN       0005   000004 SP        0003 I 010770 SUB
    0004 I 000001 SOLIT     0004   000001 SUMN      0000 R 000033 SX        0000 R 000017 SXX       0004   000003 SO
    0003   011610 TEMP      0004   000562 THIGH     0006 R 000171 TL        0004 R 001226 TLN       0000 R 000032 TLNS
    0004 R 000563 TLOW      0004   000557 TP        0004 R 000561 TMID      0005   000002 TP        0004 R 000002 TT
    0000 R 000031 TTS       0000 R 000033 TXX       0004   000576 VMIN      0005   000032 VOL       0004   000600 VPLS
```

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G001   000602 AP

      SUBROUTINE CPHS                                                        000002
C                                                                            000002
C     CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES             000002
C                                                                            000002
C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)        000002
C    * ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)         000002
      INCLUDE SPECPK                                                         000002
      COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),     /MISC/   000002
     1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT, /MISC/   000002
     2              HSUB0,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2), /MISC/   000002
     3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),/MISC/ 000002
     4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP, /MISC/ 000002
     5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV          /MISC/   000002
      COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS, /INDX/ 000002
     1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ, /INDX/ 000002
     2              NREAC,IC,J.VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE   /INDX/   000002
      COMMON /LOWTH/ NLTSP,SUBLT(40,3),TL(40,3),CPL(40,3),HL(40,3), /LOWTH/  000002
     1              SL(40,3),ILSP(40)                               /LOWTH/  000002
C                                                                            000002
         COMMON /CCC/ GRAPH,JOUT,DEMAND                                      000002
C                                                                            000002
      DATA ILP/0/,IMSG/-1/                                                   000002
      DIMENSION TXX(4),CPXX(4),HXX(4),SXX(4)                    CPHS  20     000002
      INTEGER SUM,SUBLT                                                      000002
C                                                                            000002
      IEXTND = 0                                                CPHS 190     000002
      IF(TT.LT.TLOW) IEXTND = 1                                 CPHS 200     000003
      IF(IEXTND.NE.0) IMSG = IMSG + 1                           R FEB-3      000011
      IF(IMSG.NE.0) GO TO 10                                    R FEB-3      000016
      IF(IEXTND.NE.0) WRITE(JOUT,3333) TT                                    000020
 3333 FORMAT (//25X,48HLOW TEMPERATURE THERMO EXTENSION IN CPHS AT TT =,     000031
     1        F12.6,15H DEGREES KELVIN//)                                    000031
   10 K = 1                                                                  000031
      IF (TT.LE.TMID) K=2                                       CPHS 240     000032
      KK=0                                                      CPHS 250     000040
      CPSUM=0.                                                  CPHS 260     000041
   20 IF (COEF(K,1,J).NE.0.) GO TO 30                           CPHS 270     000043
      IF (IUSE(J).LT.0) GO TO 40                                CPHS 280     000047
      KK=K                                                      CPHS 290     000053
      K=1                                                       CPHS 300     000055
      IF (KK.EQ.1) K=2                                          CPHS 310     000057
   30 IF (IEXTND .NE. 0)  GO TO 60                                           000065
   31 S(J) = ((((COEF(K,5,J)/4.0)*TT + COEF(K,4,J)/3.0)*TT + COEF(K,3,J)     000067
     1        /2.0)*TT + COEF(K,2,J))*TT + COEF(K,1,J)*TLN + COEF(K,7,J)     000067
      H0(J)=((((COEF(K,5,J)/5.)*TT+COEF(K,4,J)/4.)*TT+COEF(K,3,J)/3.)*TTCPHS 370     000114
     1+COEF(K,2,J)/2.)*TT+COEF(K,1,J)+COEF(K,6,J)/TT            CPHS 380     000114
      CPSUM=CPSUM+((((COEF(K,5,J)*TT+COEF(K,4,J))*TT+COEF(K,3,J))*TT+COECPHS 390     000140
     1F(K,2,J))*TT+COEF(K,1,J))*EN(J,NPT)                       CPHS 400     000140
   32 IF (KK .EQ. 0)  GO TO 40                                               000157
      K=KK                                                      CPHS 430     000160
      [illegible]                                               CPHS 440     000162
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00162      40  IF (J .EQ. NS)  RETURN                                                                000160
00164          J=J+1                                                             CPHS 460            000172
00165          GO TO 20                                                          CPHS 470            000174
00166      60  IF (NLISP .EQ. 0)  GO TO 31                                                           000176
00170          DO 70 IX= 1,NLISP                                                 CPHS 500            000177
00173          DO 65 KX = 1,3                                                                        000217
00176      65  IF (SUB(J,KX) .NE. SUBLT(IX,KX))  GO TO 70                                            000223
00201          GO TO 80                                                          CPHS 540            000226
00202      70  CONTINUE                                                          CPHS 550            000231
00204          GO TO 31                                                          CPHS 560            000231
00205      80  NTUP = ILSP(IX)                                                                       000233
00206          IF(TT.LT.TL(IX,1)) GO TO 90                                       CPHS 590            000235
00210          TTS = TT                                                          CPHS 600            000241
00211          TLNS= TLN                                                         CPHS 610            000243
00212          TT = TLOW                                                         CPHS 620            000245
00213          TLN= ALOG(TT)                                                     CPHS 630            000247
00214          KX = 2                                                            CPHS 640            000253
00215          SX =((((COEF(KX,5,J)/4.)*TT+COEF(KX,4,J)/3.)*TT+COEF(KX,3,J)/2.)  CPHS 650            000255
00215         1     *TT+COEF(KX,2,J))*TT+COEF(KX,1,J)*TLN+COEF(KX,7,J)           CPHS 660            000255
00216          HX =((((COEF(KX,5,J)/5.)*TT+COEF(KX,4,J)/4.)*TT+COEF(KX,3,J)/3.)  CPHS 670            000301
00216         1     *TT+COEF(KX,2,J)/2.)*TT+COEF(KX,1,J)+COEF(KX,6,J)/TT         CPHS 680            000301
00217          CPX=(((COEF(KX,5,J)*TT+COEF(KX,4,J))*TT+COEF(KX,3,J))*TT          CPHS 690            000325
00217         1     +COEF(KX,2,J))*TT+COEF(KX,1,J)                               CPHS 700            000325
00220          DO 86 KX = 1,NTUP                                                                     000351
00223          TXX(KX) = TL(IX,KX)                                                                   000351
00224          CPXX(KX) = CPL(IX,KX)                                                                 000352
00225          HXX(KX) = HL(IX,KX)                                                                   000354
00226      86  SXX(KX) = SL(IX,KX)                                                                   000356
00230          TXX(NTUP+1) = TT                                                  CPHS 770            000363
00231          CPXX(NTUP+1) = CPX                                                CPHS 780            000363
00232          HXX(NTUP+1) = HX                                                  CPHS 790            000365
00233          SXX(NTUP+1) = SX                                                  CPHS 800            000367
00234          TT = TTS                                                          CPHS 820            000371
00235          TLN = TLNS                                                        CPHS 830            000373
00236          M = 1                                                                                 000375
00237          I = 1                                                                                 000377
00240          IF (TT .LT. TXX(M))  I = -1                                                           000403
00242      87  IF (TT .GE. TXX(M) .AND. TT .LE. TXX(M+1))  GO TO 89                                  000412
00244          M = M + I                                                                             000430
00245          IF (M .LT. NTUP + 1 .AND. M .GT. 0)  GO TO 87                                         000433
00247          WRITE (JOUT,88) TT,M,NTUP,(I,TXX(I), I = 1,4)                                         000450
00261      88  FORMAT (//50X,29H*CPHS* VARIABLE OUTSIDE TABLE//45X,4HTT =,1PE15.8                    000470
00261         1,5H  M =,I2,8H  NTUP =,I2//(50X,4HTXX(,I1,3H) =,E15.8))                               000470
00262          GO TO 31                                                                              000470
00263      89  S(J) = SXX(M) + (SXX(M+1)-SXX(M))*(TT-TXX(M))/(TXX(M+1)-TXX(M))                       000472
00264          H(J) = HXX(M) + (HXX(M+1)-HXX(M))*(TT-TXX(M))/(TXX(M+1)-TXX(M))                       000506
00265          CPUSED = CPXX(M)+(CPXX(M+1)-CPXX(M))*(TT-TXX(M))/(TXX(M+1)-TXX(M))                    000514
00266          CPSUM = CPSUM + CPUSED * EN(J,NPT)                                CPHS 940            000522
00267          GO TO 32                                                          CPHS 950            000527
00270      90  IF (IEN .LT. 1)  WRITE (JOUT,900) TT                                                  000531
00271     900  FORMAT (//25X,60HERROR DURING LOW TEMPERATURE THERMO EVALUATION IN                    000542
00274         1 CPHS, TT =,F12.6,15H DEGREES KELVIN//)                                               000542
00275          IEN = 1                                                                               000547
00276          GO TO 31                                                                              000544
00277          END                                                                                   000602
END FS
```

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@FOR,S LEWIS.DELTON,LEWIS.DELTON
FOR S1E -10/25/79-17:38:09 (V,)

   SUBROUTINE DELTON       ENTRY POINT 001331

   STORAGE USED: CODE(1) 001347; DATA(0) 000201; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSTS 000006
    0004    HOLLON 000010
    0005    POINTS 000335
    0006    MISC   001204
    0007    INDA   000041
    0010    PERF   000166
    0011    OUPT   000073
    0012    CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0013    NLNOF
    0014    HEALT
    0015    OUT1
    0016    EGLOBM
    0017    OUT2
    0020    OUT3
    0021    SAVE
    0022    NROUT
    0023    NIO2$
    0024    APEN
    0025    EXP
    0026    SQRT
    0027    NIO1$
    0030    NIO3$
    0031    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    001305 1000L      0000    000035 11F        0001    000005 1306       0001    000040 1466       0001    000566 150L
    0001    000053 1546       0000    000044 190F       0000    000053 203F       0001    000255 205L       0001    000176 2146
    0000    000055 30F        0001    000451 3416       0001    000672 3526       0001    000711 3626       0001    000717 3676
    0001    000563 40L        0001    000750 4016       0001    000767 4116       0001    001004 4226       0001    001024 4336
    0001    001055 451G       0000    000114 46F        0001    001100 4646       0001    001115 4756       0000    000102 5F
    0001    001123 5026       0001    001142 5146       0001    001157 5256       0001    001176 5356       0001    001216 5465
    0000    000120 54F        0000    000123 60F        0001    000016 7L         0001    000615 860L       0000    000130 860F
    0001    001251 670L       0001    001270 902L       0000 R  000032 ALAM       0000 R  000017 ALFA       0006    000570 AN
    0006 R  000024 AM1        0006    000701 ANUM       0010    000133 APP        0003    000000 AINN       0006    000004 ATOM
    0000 R  000022 A11        0000 R  000023 A12        0000 R  000024 A21        0000 R  000025 A22        0006    000502 BO
    0000    000521 [illegible] 0000 R  000026 B1        0000 R  000027 B2         0007    000036 CALCH      0007    000001 CONVG
    0006 R  000000 CP         0005 R  000012 CFR        0006 R  000625 CPH1       0006    000564 CPSUM      0012    000002 DEMAND
     004    001167 [illegible] 0005 R  000000 ELVF1     0005 R  000047 DLTIP      0004    000000 END        0036    001263 ENSAV
    0006    000000 [illegible] 0006    001261 ENAL      0006    001262 ENSAVE     0006    001073 ENIN       0010 L  000145 EQL
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0006     000546 EQRAT     0011     000002 FA        0011     000003 FAP       0006     001112 FAZ       0011 R 000005 FB
0011     000006 FC        0011 R 000007 FCP       0011     000012 FCST      0011     000014 FCV       0011     000015 FG
0011     000017 FGL       0011     000020 FGV       0000 R 000009 FG1       0011 R 000021 FH        0011     000023 FI
0011     000025 FIV       0011 R 000027 FM        0000 R 000001 FMM       0011 R 000031 FMT       0011     000050 FN
0011 R 000052 FOUR      0006     001150 FOX       0011     000053 FP        0000 R 000003 FPP       0000 R 000002 FP1
0000 R 000004 FRA       0000 R 000005 FRB       0011     000054 FS        0011 R 000056 FSV       0011 R 000057 FT
0011     000061 FTH       0000 R 000006 FTT       0000 R 000007 FSO       0011     000063 FV        0011 R 000065 FVEL
0011 R 000001 F13       0011     000000 F9X       0000 R 000014 GAM       0005 R 000101 GAMMAS    0004     000001 GAS
0005     000001 GMLT      0010 R 000150 GMI       0012     000000 GRAPH     0007 L 000003 HP        0006     000572 HPP
0006 R 000567 HSUBO     0005 R 000000 HSUM      0010 R 000064 HI        0007     000030 IC        0007 I 000000 IDEBUG
0004     000002 IE        0000 I 000011 II        0007     000015 IMAT      0000     000143 INJP$     0000 I 000010 IOF
0007     000023 IONS      0007 I 000021 IP        0007     000037 IQSAVE    0007     000016 IQ1       0007 I 000034 IT
0000 I 000012 ITR       0004 I 000003 IZERO     0000 I 000034 J         0007     000026 JLIQ      0012 I 000001 JOUT
0007     000025 JSOL      0007     000031 JST       0007 I 000005 K         0007     000014 KMAT      0004     000004 LANK
0006     000463 LLMT      0007     000040 LSAVE     0004     000005 MOL       0007     000006 MOLES     0006 I 000626 NAME
0007     000024 NC        0007     000022 NEWR      0007     000035 NFZ       0007     000012 NLM       0007 I 000017 NOF
0007     000020 NOMIT     0007 I 000007 NP        0007 I 000011 NPT       0007 I 000027 NREAL     0007     000013 NS
0007 I 000010 NT        0006 R 000565 OF        0011 R 000067 ONE       0004     000006 OX        0006 R 001227 OXF
0005 R 000116 P         0003     000002 PATM      0010 R 000000 PCP       0006     001054 PECWT     0006 R 000563 PP
0005 R 000217 PPP       0000 R 000013 PP1       0010 R 000101 PUB       0003 R 000003 RBAR      0003 R 000004 RBR
0006     000574 RH        0006     001206 RHOF      0000 R 000020 RX        0006     001207 RMW       0010 R 000047 RRHO
0000 R 000021 RR1       0006 R 001131 RTEMP     0003     000005 RVR       0007     000033 SHOCK     0005 R 000251 SONVEL
0007     000004 SP        0005     000015 SSUM      0006     000001 SUMN      0006     000003 SO        0005 R 000157 T
0000 R 000016 TEM       0006     000562 THIGH     0011 R 000070 THREE     0006     001226 TLN       0006     000560 TLOW
0006     000557 TM        0006     000561 TMID      0005     000320 TOTN      0007 L 000002 TP        0006 R 000002 TT
0005 R 000266 TTT       0000 R 000015 TT1       0010 R 000116 TUB       0011 R 000071 TWO       0000 R 000033 UO
0005 R 000202 V         0005     000303 VLM       0006     000576 VMIN      0010 R 000032 VMOC      0007     000032 VOL
0006     000600 VPLS      0005 R 000234 WM        0006     000602 WP        0000 R 000030 X1        0000 R 000031 X2
0004     000007 ZERO      0012     000072 ZEROF
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                                                                                                                        000000
00101         1*              SUBROUTINE DETON                                                                00343900  000000
00101         2*        C                                                                                     00344000  000000
00101         3*        C     CHAPMAN-JOUGUET DETONATIONS                                                               000000
00101         4*        C                                                                                               000000
00103         5*              COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                                     /CONSTS/  000000
00104         6*              COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                               /HOLCON/  000000
00105         7*              COMMON/POINTS/PSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                               000000
00105         8*             1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                          000000
00105         9*             2 ,VLM(13),TOTN(13)                                                                        000000
00106        10*              COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),ELMT(15),BO(15),                         /MISC/  000000
00106        11*             1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                    /MISC/  000000
00106        12*             2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),                    /MISC/  000000
00106        13*             3              CP(16),AM1,CPR1,NAKE(15,5),ANUM(15,5),PECWT(15),                   /MISC/  000000
00106        14*             4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOF,                  /MISC/  000000
00106        15*             5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                             /MISC/  000000
00107        16*              COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,K,MOLES,NP,NT,NPT,NLM,NS,                     /INDX/  000000
00107        17*             1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,                 /INDX/  000000
00107        18*             2              NREAC,IC,JST,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE                   /INDX/  000000
00110        19*              COMMON /PERF/ PCP(26),VMOC(13),RRHO(13),HI(13),PUB(13),                           /PERF/  000000
00110        20*             1              TUB(13),APP(13),GMI(13),EGL                                        /PERF/  000000
00111        21*              COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),                   /OUPT/  000000
00111        22*             1              FGL,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR,               /OUPT/  000000
00111        23*             2              FP,FS(2),FSV,FT(2),FTH(2),FV(2),FVEL(2),ONE,THREE,                 /OUPT/  000000
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C-3

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00111      24*         3                 TWO,ZEROF                                        /OUPT/     000000
00111      25*     C                                                                                 000000
00112      26*            COMMON /CCC/ GRAPH,JOUT,DEMAND                                             000000
00112      27*     C                                                                                 000000
00113      28*            LOGICAL EOL,HP,TP                                                          000000
00114      29*            DATA FG1/6HGAMMA1/,FMM/6HM/M1  /,FP1/6HP1 ATM/,FPP/6HP/P1  /,              000000
00114      30*           1 FRA/6HRHO/RH/,FRB/6HO1     /,FTT/6HT/T1  /,FUD/6HDET VE/                   000000
00114      31*     C                                                                                 000000
00125      32*            XX(A,X,B,Y,C,D) = (A*X-B*Y)/(A*C-B*D)                                      000000
00125      33*     C                                                                                 000000
00126      34*            IOF = 0                                                                    000000
00127      35*            DO 4 II = 1,NREAC                                                          000000
00132      36*        4   NAME(II,5) = IZERO                                                         000005
00134      37*            TT = 0.                                                                    000007
00135      38*            IF (T(1) .LE. 0.0)  T(1) = RTEMP(1)                                        000010
00137      39*          7 IOF = IOF+1                                                                000016
00140      40*            OF = OXF(IOF)                                                              000021
00141      41*            CALL NEWOF                                                                 000023
00142      42*            WRITE(JOUT,11)                                                             000025
00144      43*         11 FORMAT(33H1DETONATION VELOCITY CALCULATIONS)                               000032
00145      44*            DO 902 IT = 1,NT                                                           000032
00150      45*            TT = T(IT)                                                                 000040
00151      46*            CALL HCALC                                                                 000042
00152      47*            CALL OUT1                                                                  000044
00153      48*            DO 902 IP=1,NP                                                             000046
00156      49*            H1(NPT) = RBAR*HSUB0                                                       000055
00157      50*            TUB(NPT) = T(IT)                                                           000061
00160      51*            PUB(NPT) = P(IP)                                                           000063
00161      52*            CP(NPT) = RBAR*CPR1                                                        000065
00162      53*            ITR= 0                                                                     000070
00163      54*            TT= 3800.                                                                  000071
00164      55*            PP1= 15.                                                                   000073
00165      56*            PP = PP1*P(IP)                                                             000075
00166      57*            HSUB0 = H1(NPT)/RBAR + 0.750*T(IT)*PP1/AM1                                 000077
00167      58*            TP = .FALSE.                                                               000105
00170      59*            HP= .TRUE.                                                                 000106
00171      60*            CALL EQLBRM                                                                000110
00172      61*            HSUB0 = H1(NPT)/RBAR                                                       000117
00173      62*            HP= .FALSE.                                                                000122
00174      63*            IF (TT .LE. 0.0)  GO TO 902                                                000123
00176      64*            GAM= GAMMAS(NPT)                                                           000126
00177      65*            TT1 = TT/T(IT)                                                             000137
00200      66*            II= 0                                                                      000142
00201      67*            TEM=TT1-.75*PP1/(CPR(NPT)*AM1)                                             000143
00202      68*            WRITE(JOUT,190)TT                                                          000157
00205      69*        190 FORMAT(8HOT EST.=,F8.2/11X,4HP/P1,17X,4HT/T1)                              000160
00206      70*            WRITE(JOUT,203) II,PP1,TT1                                                 000160
00213      71*            DO 202 II = 1,3                                                            000176
00216      72*            ALFA = WM(NPT)/AM1/TT1                                                     000176
00217      73*            PP1= (1.+GAM)*(1.+(1.-4.*GAM*ALFA/(1.+GAM)**2)**.5)/(2.*GAM*ALFA)          000201
00220      74*            RK=PP1*ALFA                                                                000220
00221      75*            TT1= TEM+.5*PP1*GAM*(RK*RK-1.)/(AM1*CPR(NPT)*RK)                           000222
00222      76*        202 WRITE(JOUT,203) II,PP1,TT1                                                 000235
00230      77*        203 FORMAT (I5,2E20.8)                                                         000247
00231      78*            TP= .TRUE.                                                                 000247
00232      79*            TT = TT1*T(IT)                                                             000251
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00233     205 ITR= ITR+1                                                          000255
00234         PP = PP1*P(IP)                                                      000257
00235         CALL EQLBRM                                                         000262
00236         IF (NPT.EQ.0) GO TO 1000                                            000264
00240         IF (TT .LE. 0.0)  GO TO 860                                         000266
00242         GAM= GAMMAS(NPT)                                                    000272
00243         RR1 = PP1*WM(NPT)/AM1/TT1                                           000274
00244         A11= 1./PP1 + GAM*RR1*DLVPT(NPT)                                    000302
00245         A12= GAM*RR1*DLVTP(NPT)                                             000310
00246         A21= .5*GAM*(RR1**2-1.-DLVPT(NPT)*(1.+RR1**2))+DLVTP(NPT)-1.        000314
00247         A22=-.5*GAM*DLVTP(NPT)*(RR1**2+1.)-WM(NPT)*CPR(NPT)                 000330
00250         B1= 1./PP1-1.+GAM*(RR1-1.)                                          000343
00251         B2 = WM(NPT)*(HSUM(NPT) - H1(NPT)/RBAR)/TT - 0.5*GAM*(RR1**2 - 1.)  000353
00252         X1 = XX(A22,B1,A12,B2,A11,A21)                                      000370
00253         X2 = XX(A11,B2,A21,B1,A22,A12)                                      000400
00254         ALAM= 1.                                                            000412
00255         TEM = X1                                                            000414
00256         IF(TEM.LT.0.)  TEM = -TEM                                           000416
00260         IF(X2.GT.TEM)  TEM=X2                                               000423
00262         IF (-X2.GT.TEM) TEM = -X2                                           000431
00264         IF(TEM.GT.0.4) ALAM=.4/TEM                                          000437
00266         PP1= PP1*EXP(X1*ALAM)                                               000446
00267         TT1= TT1*EXP(X2*ALAM)                                               000456
00270         TT = TT1*T(IT)                                                      000466
00271         UD = RR1*SQRT(RBR*GAM*TT/WM(NPT))                                   000470
00272         WRITE(JOUT,30)ITR,PP1,TT1,RR1,X1,X2                                 000503
00302      30 FORMAT(7H0ITER =,I2,5X,6HP/P1 =,E15.8,5X,6HT/T1 =,E15.8,5X,10HRHO/  000516
00302        1RHO1 =,E15.8/7X,13HDEL LN P/P1 =,E15.8,5X,13HDEL LN T/T1 =,E15.8)   000516
00302     C   CONVERGENCE TEST                                                    000516
00303         IF(ITR.LE.10 .AND. TEM.GT.0.5E-04)  GO TO 205                       000516
00305         RRHO(NPT)=RR1                                                       000534
00306         IF (CP(NPT) .LE. 0.0)  GO TO 40                                     000536
00310         GM1(NPT) = CP(NPT)/(CP(NPT) - RBAR/AM1)                             000541
00311         VMOC(NPT) = UD/SQRT(RBR*GM1(NPT)*T(IT)/AM1)                         000547
00312         GO TO 150                                                           000561
00313      40 GM1(NPT) = 0.                                                       000563
00314         VMOC(NPT) = 0.                                                      000564
00315     150 K = 0                                                               000566
00316         IF (IP .EQ. NP .AND. IT .EQ. NT .OR. TT .LE. 0.0)  GO TO 860        000566
00320         K = NPT                                                             000610
00321         IF(NPT.NE.13)  GO TO 870                                            000612
00321     C   OUTPUT                                                              000612
00323     860 WRITE(JOUT,5)                                                       000615
00325       5 FORMAT(1H1,42X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS )  000621
00326         CALL OUT1                                                           000621
00327         WRITE(JOUT,46)                                                      000623
00331      46 FORMAT(13H UNBURNED GAS//)                                          000633
00332         FMT(3) = F13                                                        000633
00333         FMT(4) = FOUR                                                       000635
00334         WRITE(JOUT,FMT) FP1,FB,FB,(PUB(J), J = 1,NPT)                       000637
00345         FMT(4) = TWO                                                        000654
00346         WRITE(JOUT,FMT) FT,FB,(TUB(J), J = 1,NPT)                           000656
00356         WRITE(JOUT,FMT) FH,FB,(H1(J), J = 1,NPT)                            000675
00366         DO 56 J = 1,NPT                                                     000717
00371         V(J) = AM1                                                          000717
00372      56 SONVEL(J) = SQRT(RBR*GM1(J)*TUB(J)/AM1)                             000720
```

```
00374          FMT(4) = THREE                                          000732
00375          WRITE(JOUT,FMT) FM,FB,(V(J), J = 1,NPT)                 000734
00405          FMT(4) = FOUR                                           000753
00406          WRITE(JOUT,FMT) FCP,(CP(J), J = 1,NPT)                  000755
00415          WRITE(JOUT,FMT) FG1,FB,FB,(GM1(J), J = 1,NPT)           000772
00426          FMT(4) = ONE                                            001007
00427          WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(J), J = 1,NPT)         001011
00437          WRITE(JOUT,58)                                          001027
00441       58 FORMAT(11H0BURNED GAS//)                                001034
00442          FMT(3) = ONE                                            001034
00443          CALL OUT2                                               001036
00444          WRITE(JOUT,68)                                          001040
00446       68 FORMAT(22H0DETONATION PARAMETERS //)                    001050
00447          FMT(4) = THREE                                          001050
00450          DO 70 J = 1,NPT                                         001055
00453          V(J) = PPP(J)/PUB(J)                                    001055
00454          PCP(J) = TTT(J)/TUB(J)                                  001057
00455     70   SONVEL(J) = SONVEL(J)*RRHO(J)                           001062
00457          WRITE(JOUT,FMT) FPP,FB,FB,(V(J), J = 1,NPT)             001066
00470          WRITE(JOUT,FMT) FTT,FB,FB,(PCP(J), J = 1,NPT)           001103
00501          DO 73 J = 1,NPT                                         001123
00504     73   V(J) = WM(J)/AM1                                        001123
00506          FMT(4) = FOUR                                           001126
00507          WRITE(JOUT,FMT) FMM,FB,FB,(V(J), J = 1,NPT)             001130
00520          WRITE(JOUT,FMT) FRA,FRB,FB,(RRHO(J), J = 1,NPT)         001145
00531          WRITE(JOUT,FMT) FM,FB,(VMOC(J), J = 1,NPT)              001162
00541          FMT(4) = ONE                                            001201
00542          WRITE(JOUT,FMT) FUD,FVEL,(SONVEL(J), J = 1,NPT)         001203
00552          EQL=.TRUE.                                              001221
00553          CALL OUT3                                               001223
00554          IF (K .EQ. 0 .AND. IOF .EQ. NOF)  GO TO 1000            001225
00556          IDEBUG = IDEBUG-13                                      001237
00557          WRITE(JOUT,868)                                         001242
00561      868 FORMAT(1H1)                                             001247
00562          NPT = 0                                                 001247
00563      870 NPT = NPT + 1                                           001251
00564          IF (K .EQ. 1)  K = -1                                   001253
00566          CALL SAVE                                               001260
00567          WRITE(JOUT,868)                                         001262
00571      902 CONTINUE                                                001274
00574          IF(IOF.GE.NOF)  GO TO 1000                              001274
00576          IDEBUG = IDEBUG+13                                      001300
00577          GO TO 7                                                 001303
00600     1000 TF = .FALSE.                                            001305
00601          RETURN                                                  001305
00602          END                                                     001346
END FOR
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@FOR,S LEWIS.EQLBRM,LEWIS.EQLBRM
FOR  ES -10/25/79-17:38:12 (9,)

   SUBROUTINE EQLBRM    ENTRY POINT 003112

   STORAGE USED: CODE(1) 003130; DATA(0) 000440; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003     CONSTS 000006
    0004     MOLCON 000310
    0005     POINTS 000335
    0006     SPECES 012120
    0007     MISC   001264
    0010     DOUBLE 001560
    0011     INDX   000041
    0012     PERF   000166
    0013     CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0014     CPHS
    0015     MATRIX
    0016     GAUSS
    0017     ALOG
    0020     NWDU$
    0021     NIO1$
    0022     NIO2$
    0023     EXP
    0024     NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001     001202 100L       0001     001211 101L       0001     002164 1023G      0001     002214 1033G      0000     000201 110F
    0001     001452 111L       0001     001575 1115L      0001     001633 1116L      0001     001517 113L       0001     002475 1130G
    0001     002503 1134G      0001     001513 114L       0001     001542 115L       0001     002543 1150G      0001     001660 116L
    0001     002616 1160L      0001     002446 1165L      0001     002710 1171L      0000     000202 1183F      0001     002636 1201G
    0001     002670 1217G      0001     002733 1240G      0001     002046 13L        0001     001747 130L       0000     000300 136F
    0001     002652 143L       0000     000236 144F       0001     002255 147L       0001     002262 148L       0001     000116 151G
    0001     002510 153L       0001     002304 154L       0000     000244 156F       0001     002334 157L       0001     002373 158L
    0001     002431 159L       0001     002144 160L       0000     000256 161F       0001     000151 165G       0001     002622 165L
    0001     002642 166L       0000     000266 168F       0001     002610 169L       0001     002613 170L       0001     002717 171L
    0000     000077 172F       0001     000430 174L       0001     002002 183L       0001     003005 186L       0000     000153 1924F
    0001     002774 199L       0000     000305 201F       0001     001561 2115L      0001     000244 221G       0001     000277 232G
    0000     000260 244F       0001     000325 245G       0001     000332 251G       0001     000374 270G       0001     000406 277G
    0000     000206 306F       0001     000464 315G       0001     000517 324G       0001     000131 33L        0001     000613 360G
    0000     000071 373F       0001     002645 40L        0001     000721 416G       0001     000732 422G       0001     000155 43L
    0001     001003 445G       0001     001141 477G       0001     000125 499L       0001     001172 506G       0001     001257 531G
    0001     001413 600G       0001     002313 62L        0001     000251 63L        0001     001464 631G       0001     000302 67L
    0001     001425 673G       0001     001642 704G       0001     000342 72L        0001     001722 726G       0000     000075 73F
    0000     000126 74F        0001     001760 744G       0000     000303 771F       0000     000063 772F       0001     000412 773L
    0001     000524 774L       0001     002536 775L       0000     000132 776F       0001     000747 80L        0001     000766 83L
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0001      001023 84L       0001      001036 85L       0001      000571 871L      0001      003063 873L      0000      000105 874F
0001      001332 917L      0000      000134 923F      0000      000157 924F      0000      000176 925F      0001      000603 966L
0001      000622 968L      0001      000632 969L      0001      001111 97L       0001      000635 970L      0001      000644 971L
0000      000220 973F      0001      000654 997L      0006 R    006034 A         0000 R    000047 AA        0012      000150 AEAT
0007      000570 AM        0000 R    000042 AMBDA     0000 R    000043 AMBDA1    0007      000624 AM1       0007      000741 ANUM
0012 R    000133 APP       0003      000000 ATMN      0007      000004 ATOM      0007 R    000502 BO        0007      000521 BOP
0011      000036 CALCH     0006      000000 COEF      0011 L    000001 CONVG     0005 R    000032 CPR       0007      000625 CPR1
0007 R    000564 CPSUM     0000 R    000026 CRITV     0007      000604 DATA      0000 R    000055 DELF      0006 R    005670 DELN
0013      000002 DEMAND    0007      001167 DENS      0000 R    000041 DLNT      0005 R    000064 DLVPT     0005 R    000047 DLVTP
0006 R    002734 EN        0004      000000 END       0000 R    000025 ENL       0006 R    005360 ENLN      0007      001263 ENLSAV
0007 R    000000 ENN       0007 R    001261 ENNL      0007      001262 ENSAVE    0000 R    000033 ENSOL     0007      001073 ENTH
0012      000165 EQL       0007 R    000566 EQRAT     0007      001112 FAZ       0000 R    000045 FNEG1     0000 R    000046 FNEG2
0007      001150 FOX       0010 D    000000 G         0005 R    000101 GAMMAS    0004      000001 GAS       0003      000001 GMET
0013      000000 GRAPH     0011 L    000003 HP        0007      000572 HPP       0007      000567 HSUBO     0005 R    000000 HSUM
0005 R    005524 HO        0000 I    000032 I         0011 L    000030 IC        0011 I    000000 IDEBUG    0004 I    000002 IE
0011 I    000015 IMAT      0000 I    000051 INC       0000      000400 INJP$     0011 L    000023 IONS      0011      000021 IP
0011      000037 IOSAVE    0011 I    000016 I01       0000 I    000035 IO2       0000 L    000022 ISING     0011      000005 ISV
0011      000034 IT        0000 I    000030 ITNUMB    0006 I    011444 IUSE      0004      000003 IZERO     0000 I    000031 J
0000 I    000056 JDELF     0000 I    000037 JJ        0000 I    000053 JKG       0011 I    000026 JLIQ      0013 I    000001 JOUT
0011 I    000025 JSOL      0011 I    000031 JS1       0000 I    000052 KG        0011 I    000014 KMAT      0011 I    000012 L
0004      000004 LANK      0007 I    000463 LLMT      0000 L    000023 LOGV      0011      000040 LSAVE     0004      000005 MOL
0011      000006 MOLES     0007      000626 NAME      0011 I    000024 NC        0000 I    000040 NEN       0011      000022 NEWR
0011      000035 NFZ       0011      000017 NOF       0011      000020 NOMIT     0011      000007 NP        0011 I    000011 NPT
0011      000027 NREAC     0011 I    000013 NS        0000 I    000000 NSPP1     0011      000010 NT        0000 I    000036 NTZERO
0000 I    000034 NUMR      0007      000565 OF        0004      000006 OX        0007      001227 OXF       0005      000116 P
0003      000002 PATM      0012      000000 PCP       0007      001054 PECWT     0007 R    000563 PP        0005 R    000217 PPP
0000 R    000001 PROW      0003      000003 RBAR      0003      000004 RBR       0007      000574 RH        0007      001206 RHOP
0000 L    000024 RITE      0007      001207 RMW       0007      001131 RTEMP     0003 R    000005 RVR       0006 R    002570 S
0011 L    000033 SHOCK     0000 R    000027 SIZEF     0006      011754 SLN       0005      000251 SONVEL    0011 L    000004 SP
0012      000047 SPIM      0000 R    000050 SS        0005 R    000015 SSUM      0006 R    010770 SUB       0012      000101 SUBAR
0000 D    000020 SUM       0007 R    000001 SUMN      0000 R    000044 SUM1      0012      000116 SUPAR     0007 R    000003 SO
0005 R    000150 T         0006 R    011610 TEMP      0007 R    000562 THIGH     0007 R    001226 TLN       0007 R    000560 TLOW
0007 R    000557 TM        0000 R    000054 TMELT     0007      000561 TMID      0000 R    000057 TN        0005 R    000320 TOTN
0011 L    000002 TP        0007 R    000002 TT        0005 R    000266 TTT       0005      000202 V         0012      000064 VACI
0005 R    000303 VLM       0007      000576 VMIN      0012      000032 VMOC      0011 L    000032 VOL       0007      000600 VPLS
0005 R    000234 WM        0007      000602 WP        0010 D    001510 X         0004      000007 ZERO



00101      1*            SUBROUTINE EQLBRM                                             EQLN0002    000000
00101      2*     C                                                                                000000
00101      3*     C   ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES      EQLN0003    000000
00101      4*     C                                                                    EQLN0004    000000
00103      5*            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                   /CONSTS/    000000
00104      6*            COMMON /MOLCON/ ENO,GAS,IE,IZERO,LANK,MOL,OX,ZERO             /MOLCON/    000000
00105      7*            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)               000000
00105      8*           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)          000000
00105      9*           2 ,VLM(13),TOTN(13)                                                        000000
00105     10*     C      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)           000000
00105     11*     C     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)            000000
00106     12*            INCLUDE SPECPR                                                            000000
00112     13*            COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),       /MISC/    000000
00112     14*           1                BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT, /MISC/    000000
00112     15*           2                HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2), /MISC/    000000
00112     16*           3                DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15), /MISC/ 000000
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00112        4          ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,     /MISC/      000000
00112        5          RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                /MISC/      000000
00113         COMMON /DOUBLE/ G(20,21), X(20)                                EQLN0013    000000
00114         COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,  /INDX/      000000
00114        1          KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,    /INDX/      000000
00114        2          NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE      /INDX/      000000
00115         COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),    /PERF/      000000
00115        1          SUPAR(13),APP(13),AEAT(13),EQL                        /PERF/      000000
00115   C                                                                                 000000
00116            COMMON /CCC/ GRAPH,JOUT,DEMAND                                           000000
00116   C                                                                                 000000
00117         DIMENSION PROW(15)                                                          000000
00120         DOUBLE PRECISION G,SUM,X                                                    000000
00121         LOGICAL CONVG,HP,IC,IONS,ISING,LOGV,RITE,SHOCK,SP,TP,VOL                    000000
00121   C                                                                                 000000
00122         LNL = LNNL                                                                  000003
00123         RITE = .FALSE.                                                              000001
00124         IF(IDEBUG.GT.0.AND.NPT.GE.IDEBUG)  RITE=.TRUE.                              000002
00126         CRITV = 5.0E-6                                                              000021
00127         SIZEF = 0.                                                                  000023
00130         ISING = .FALSE.                                                             000024
00131         LOGV = .FALSE.                                                              000025
00132         IF (VOL)  PP = RVR*ENN*TT/VLM(NPT)                                          000026
00134         TLN = ALOG(TT)                                                              000040
00135         CONVG = .FALSE.                                                             000044
00136         ITNUMB = 100                                                                000045
00137         JS1 = 1                                                                     000047
00140         CALL CPHS                                                                   000051
00141         TM = ALOG(PP/ENN)                                                           000053
00141   C     IF(IC) PREVIOUS POINT HAD SINGULAR MATRIX                                   000053
00142         IF(IC)  GO TO 966                                                           000062
00144         IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33                                    000064
00146         L = L+1                                                                     000102
00147         IQ1 = IQ1+1                                                                 000105
00150         DO 499 J = 1,NS                                                             000116
00153         IF (A(L,J) .EQ.0.) GO TO 499                                                000116
00155         EN(J,NPT) = 1.E-8                                                           000117
00156         ENLN(J) = -18.420681                                                        000121
00157         IUSE(J) = 0                                                                 000123
00160     499 CONTINUE                                                                    000131
00162      33 IF(NPT.EQ.1.AND..NOT.SHOCK)  WRITE(JOUT,244)(LLMT(I),I=1,L)                 000131
00171     244 FORMAT (4HOPT ,14(5X,A4))                                                   000155
00171   C     BEGIN ITERATION                                                             000155
00172      43 IF(IC)  GO TO 1171                                                          000155
00174         IF (.NOT.CONVG)  GO TO 62                                                   000156
00176         SUMN = ENN                                                                  000166
00177         IF(JSOL.EQ.0)  GO TO 62                                                     000170
00201         ENSOL = EN(JSOL,NPT)                                                        000172
00202         EN(JSOL,NPT) = EN(JSOL,NPT)+EN(JLIQ,NPT)                                    000176
00203         IUSE(JLIQ) = -IUSE(JLIQ)                                                    000200
00204         IQ1 = IQ1-1                                                                 000202
00205         DLVTP(NPT) = 0.                                                             000205
00206         CPR(NPT) = 0.                                                               000206
00207         GAMMAS(NPT) = 0.                                                            000207
00210         LOGV = .TRUE.                                                               000210
00211      62 CALL MATRIX                                                    EQLN0048    000213
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00212     73*          NUMB = IQ1 - ITNUMB                                                 000214
00213     74*          IQ2 = IQ1 + 1                                                       000217
00214     75*          IF(.NOT.CONVG)     GO TO 67                                         000222
00216     76*          IF (LOGV.AND.JSOL.EQ.0) GO TO 63                                    000224
00220     77*          DO 182  I=1,L                                         EQLNU140      000244
00223     78*     182  PROW(I) = G(IQ1,I)                                                  000244
00225     79*          IF (.NOT.LOGV) GO TO 67                                             000246
00225     80*    C     LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT                    000246
00227     81*       63 G(IQ1,IQ2) = ENN                                                    000251
00230     82*          J = IQ1 - 1                                                         000260
00231     83*          DO 777 I = 1,J                                                      000270
00234     84*     777  G(I,IQ2) = G(I,IQ1)                                                 000277
00236     85*       67 IF(.NOT.RITE)  GO TO 72                                             000302
00240     86*          WRITE(JOUT,772) NUMB                                                000303
00243     87*      772 FORMAT (11H0ITERATION  ,I3,6X,7HMATRIX //)                          000325
00244     88*          DO 911 I=1,IMAT                                       EQLNU051      000325
00247     89*     911  WRITE(JOUT,73) (G(I,J), J = 1,KMAT)                                 000325
00256     90*       72 IF(CONVG)  IMAT=IMAT-1                                              000342
00260     91*          J = IMAT                                                            000346
00261     92*          CALL GAUSS                                                          000350
00262     93*          IF (J .NE. IMAT)  GO TO 774                                         000352
00264     94*          IF(.NOT.RITE)  GO TO 773                                            000355
00265     95*          WRITE(JOUT,373)(LLMT(I),I=1,L)                                      000363
00274     96*      373 FORMAT (7H0PI     ,9(A4,10X))                                       000377
00275     97*          WRITE(JOUT,73)(X(I),I=1,IMAT)                                       000377
00303     98*       73 FORMAT (9E14.6)                                       EQLNU062      000412
00304     99*      773 IF(.NOT.CONVG)  GO TO 85                                            000412
00306    100*          IF(.NOT.LOGV)  GO TO 174                                            000413
00310    101*          IF(JLIQ.NE.0) EN(JSOL,NPT)=ENSOL                                    000421
00312    102*          GO TO 171                                                           000426
00313    103*      174 SUM = 0.                                              EQLNU148      000430
00314    104*          DO 175 J=1,L                                          EQLNU149      000431
00317    105*     175  SUM = SUM + PROW(J)*X(J)                                            000464
00321    106*          DLVTP(NPT) = 1.+G(IQ2,IQ1)/ENN-SUM/ENN  - X(IQ1)      EQLNU151      000470
00322    107*          CPR(NPT) = G(IQ2,IQ2)                                 EQLNU152      000502
00323    108*          DO 176 J=1,IQ1                                        EQLNU153      000512
00326    109*     176  CPR(NPT) = CPR(NPT) - G(IQ2,J)*X(J)                                 000512
00330    110*          LOGV = .TRUE.                                         EQLNU155      000520
00331    111*          GO TO 62                                                            000522
00331    112*    C   SINGULAR MATRIX                                                       000522
00332    113*      774 IF(.NOT.CONVG)  GO TO 775                                           000524
00332    114*    C     IF(ISING)  SINGULAR ONCE                                            000524
00332    115*    C     IF(IC)     SINGULAR TWICE                                           000524
00334    116*          WRITE(JOUT,172)                                                     000525
00336    117*      172 FORMAT(28H0DERIVATIVE MATRIX SINGULAR )                             000532
00337    118*          IC = .TRUE.                                                         000532
00340    119*          GO TO 1171                                                          000534
00341    120*      775 IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 871        000536
00343    121*          WRITE(JOUT,874)                                                     000562
00345    122*      874 FORMAT(96H0LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE    000567
00345    123*         1BEEN INCLUDED ON AN INSERT CARD, RESTART )                          000557
00346    124*          GO TO 873                                                           000567
00347    125*      871 WRITE(JOUT,74)                                                      000571
00351    126*       74 FORMAT(16H0SINGULAR MATRIX)                                         000575
00352    127*          IF(IC)  GO TO 873                                                   000575
00354    128*          IF (ISING) GO TO 997                                                000577
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00356    129*          NTZERO = 0                                                          000601
00357    130*      966 DO 970 JJ = 1, NS                                                   000603
00362    131*          IF(IUSE(JJ)) 970,968,967                                            000613
00365    132*     967  IF (EN(JJ,NPT))  969,873,969                                        000616
00370    133*     968  IF (EN(JJ,NPT) .GT. 0.0)  GO TO 969                                 000622
00372    134*          EN(JJ,NPT) = 1.0E-6                                                 000624
00373    135*          ENLN(JJ) = -13.815511                                               000626
00374    136*          GO TO 970                                                           000630
00375    137*      969 NTZERO = NTZERO+1                                                   000632
00376    138*      970 CONTINUE                                                            000637
00400    139*          IF(.NOT.IC)  GO TO 971                                              000637
00402    140*          IC = .FALSE.                                                        000641
00403    141*          GO TO 43                                                            000642
00404    142*      971 ISING = .TRUE.                                                      000644
00405    143*          WRITE(JOUT,776)                                                     000645
00407    144*      776 FORMAT (8H0RESTART)                                                 000652
00410    145*          GO TO 43                                                            000652
00411    146*     997  IF(NTZERO.NE.L-1.OR.EQRAT.GT.1.00001.OR.EQRAT.LT..99999) GO TO 873  000654
00413    147*          ENN=0.                                                              000710
00414    148*          NEN = 0                                                             000711
00415    149*          DO 83  I=1,L                                                        000721
00420    150*          JJ = 0                                                              000724
00421    151*          DO 80  J=1,NS                                                       000732
00424    152*          IF (EN(J,NPT) .EQ. 0.0 .OR. A(I,J) .EQ. 0.0)  GO TO 80              000732
00426    153*          IF (JJ .NE. 0)  GO TO 83                                            000742
00430    154*          JJ = J                                                              000744
00431    155*       80 CONTINUE                                                            000752
00433    156*          NEN = NEN+1                                                         000752
00434    157*          EN(JJ,NPT) = B0(I)/A(I,JJ)                                          000755
00435    158*       83 CONTINUE                                                            000767
00437    159*          IF(NEN.LT.NTZERO)  GO TO 873                                        000767
00441    160*          CONVG = .TRUE.                                                      000773
00442    161*          IC = .TRUE.                                                         000775
00443    162*          HSUM(NPT) = 0.                                                      000776
00444    163*          DO 84  J=1,NS                                                       001003
00447    164*          IF (EN(J,NPT) .LE. 0.0)  GO TO 84                                   001003
00451    165*          ENN = EN(J,NPT)+ENN                                                 001005
00452    166*          ENLN(J) = ALOG(EN(J,NPT))                                           001010
00453    167*          HSUM(NPT) = HSUM(NPT) + EN(J,NPT)*H0(J)                             001016
00454    168*       84 CONTINUE                                                            001025
00456    169*          TM = ALOG(PP/ENN)                                                   001025
00457    170*          GO TO 43                                                            001034
00460    171*       85 ITNUMB= ITNUMB-1                                        EQLN0068    001036
00461    172*          IF (ITNUMB .LT. 30)  CRITV = CRITV * 2.50E-7                        001040
00461    173*    C     OBTAIN CORRECTIONS TO THE ESTIMATES                     EQLN0070    001040
00463    174*          JJ = L + 1                                                          001047
00464    175*          IF(VOL)  X(IC2)=X(IC1)                                              001060
00466    176*          IF(TP)  X(IC2)=0.                                                   001066
00470    177*          DLNT= X(IC2)                                            EQLN0072    001073
00471    178*          SUM = X(IC1)                                                        001076
00472    179*          IF(.NOT.VOL) GO TO 97                                               001101
00474    180*          X(IC1) = 0.                                                         001103
00475    181*          SUM =    -DLNT                                                      001105
00476    182*       97 DO 101 J=1,NS                                                       001111
00501    183*          IF (IUSE(J)) 101,98,100                                             001145
00503    184*       98 DELN(J) = H0(J)*DLNT-H0(J)*S(J)-ENLN(J)-TM*SUM                      001151
```

```
00505          DO 99 I = 1,L                                                                      001172
00510     99   DELN(J) = DELN(J) + A(I,J)*X(I)                                                    001172
00512          GO TO 101                                                                          001200
00513    100   DELN(J) = X(JJ)                                                                    001202
00514          JJ = JJ + 1                                                                        001205
00515    101 CONTINUE                                                                  EQLNU079   001213
00517          AMBDA= 1.                                                               EQLNU080   001213
00520          AMBDA1= 1.                                                              EQLNU081   001215
00521          SUM = X(101)                                                                       001216
00522          IF(SUM.LT.0.)  SUM=-SUM                                                            001222
00524          IF(DLNT.GT.SUM)  SUM=DLNT                                                          001230
00526          IF(-DLNT.GT.SUM)  SUM=-DLNT                                                        001236
00530          DO 917 J=1,NS                                                           EQLNU084   001252
00533          IF (IUSE(J).NE.0) GO TO 917                                                        001252
00535          IF (EN(J,NPT) .GT. 0.0 .AND. DELN(J) .GT. SUM)  SUM = DELN(J)                      001253
00537          IF (EN(J,NPT) .GT. 0.0 .OR. DELN(J) .LE. 0.0)  GO TO 917                           001272
00541          SUM1 = (-9.212-ENLN(J)+ ENL)/(DELN(J)-X(101))                                      001306
00542          IF(SUM1.LT.0.)  SUM1=-SUM1                                                         001316
00544          IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1                                                  001323
00546    917 CONTINUE                                                                  EQLNU089   001334
00550          IF(SUM.GT.2.)AMBDA=2./SUM                                               EQLNU090   001334
00552          IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1                                                001344
00554          IF(.NOT.RITE)  GO TO 111                                                           001352
00556          WRITE(JOUT,923) TT,ENN, ENL,PP,TM,AMBDA                                            001354
00566    923 FORMAT (3HOT=,E15.8,6H  ENN=,E15.8,7H  ENNL=E15.8,5H  PP=,E15.8,                     001367
00566       1 9H  LN P/N=E15.8,8H  AMBDA=E15.8 )                                                  001367
00567          IF(VOL)  WRITE(JOUT,1924) VLM(NPT)                                                 001367
00573   1924 FORMAT(8H VOLUME=,E15.8,2HCC)                                                        001401
00574          WRITE(JOUT,924)                                                                    001401
00576    924 FORMAT(1H0,16X,2HNI,12X,5HLN NI,8X,9HDEL LN NI,10X,4HH/RT,9X,4HSO/                   001413
00576       1R,12X,6H-G0/RT,9X,5H-G/RT  )                                                         001413
00577          DO 926 J=1,NS                                                                      001413
00602          FNEG1 = S(J)-H0(J)                                                                 001413
00603          FNEG2 = FNEG1                                                                      001415
00604          IF(IUSE(J).EQ.0)  FNEG2=FNEG2-ENLN(J)-TM                                           001416
00606    926  WRITE(JOUT,925) SUB(J,1),SUB(J,2),SUB(J,3),EN(J,NPT),ENLN(J),                       001424
00606       A                 DELN(J),H0(J),S(J),FNEG1,FNEG2                                      001424
00623    925 FORMAT (1X,3A4,7E15.6)                                                               001444
00624          WRITE(JOUT,110)                                                                    001444
00626    110 FORMAT(1H0)                                                                          001452
00626   C      APPLY CORRECTIONS TO ESTIMATES                                          EQLNU096   001452
00627    111 SUM = 0.                                                                             001452
00630          DO 113 J=1,NS                                                           EQLNU099   001453
00633          IF (IUSE(J)) 113,112,114                                                           001464
00636    112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)                                             EQLNU100   001467
00637          EN(J,NPT) = 0.                                                          EQLNU101   001473
00640          IF (ENLN(J) + 18.4206810 .LE. ENL)  GO TO 113                                      001474
00642          EN(J,NPT) = EXP(ENLN(J))                                                           001500
00643          SUM = SUM+EN(J,NPT)                                                                001506
00644          GO TO 113                                                                          001511
00645    114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)                                              001513
00646    113 CONTINUE                                                                             001521
00650          SUMN = SUM                                                                         001521
00651          IF (TP) GO TO 115                                                       EQLNU104   001523
00653          TLN= TLN+AMBDA*DLNT                                                     EQLNU105   001525
00654          TT      = EXP(TLN)                                                      EQLNU106   001531
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00655            JS1 = 1                                                                001535
00656            CALL CPHS                                                              001537
00657        115 IF(VOL) GO TO 2115                                                     001542
00661            ENL = ENL+AMBDA*X(IQI)                                                 001543
00662            ENN = EXP(ENL)                                                         001553
00663            GO TO 1115                                                             001557
00664       2115 ENN = SUMN                                                             001561
00665            ENNL = ALOG(ENN)                                                       001562
00666            PP = RVR*TT*ENN/VLM(NPT)                                               001566
00667       1115 TM = ALOG(PP/ENN)                                                      001575
00670            IF (LLMT(L).NE.IE) GO TO 116                                           001603
00670      C     CHECK ON REMOVING IONS                                                 001603
00672            DO 1116 J = 1,NS                                                       001625
00675            IF (A(L,J).EQ.0.) GO TO 1116                                           001625
00677            IF (EN(J,NPT).GT.0.) GO TO 116                                         001627
00701       1116 CONTINUE                                                               001642
00703            DO 1118  J=1,NS                                                        001642
00706      1118  IF (A(L,J) .NE. 0.0)  IUSE(J) = - 10000                                001642
00711            L = L-1                                                                001650
00712            IQ1 = IQ1-1                                                            001653
00713            GO TO 43                                                               001656
00713      C     TEST FOR CONVERGENCE                                      EQLNU110     001656
00714        116 IF (ITNUMB.EQ.0) GO TO 13                                 EQLNU112     001660
00716            IF (AMBDA.LT.1.) GO TO 43                                 EQLNU113     001661
00720            SUM = (ENN-SUMN)/ENN                                                   001674
00721            IF (SUM.LT.0.) SUM = -SUM                                              001704
00723            IF (SUM .GT. CRITV)  GO TO 43                                          001712
00725            DO 130 J=1,NS                                             EQLNU115     001722
00730            IF (IUSE(J).LT.0) GO TO 130                                            001722
00732            AA= DELN(J)/SUMN                                                       001725
00733            IF(AA.LT.0.)  AA=-AA                                                   001730
00735            IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)                                    001735
00737            IF (AA .GT. CRITV)  GO TO 43                                           001742
00741        130 CONTINUE                                                               001751
00741      C     CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS                    001751
00743            TOTN(NPT) = 0.                                                         001751
00744            SSUM(NPT) = 0.                                                         001753
00745            DO 183 J=1,NS                                             EQLNU133     001760
00750            IF(IUSE(J).LT.0)  GO TO 183                                            001760
00752            TOTN(NPT) = TOTN(NPT) + EN(J,NPT)                                      001762
00753            SS = S(J)                                                              001765
00754            IF(IUSE(J).EQ.0)  SS=SS-ENLN(J)-TM                                     001767
00756            SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)                                     001775
00757        183 CONTINUE                                                  EQLNU136     002004
00761            IF(.NOT.SP.OR.NPT.EQ.1)  GO TO 13                                      002004
00763            SS = SSUM(NPT) -S0                                                     002014
00764            IF(SS.LT.(-0.00005).OR.SS.GT.0.00005)  GO TO 43                        002020
00766            IF(RITE)  WRITE(JOUT,1183)  SS                                         002035
00772       1183 FORMAT(11H0DELTA S/R =,E15.8)                                          002046
00773         13 CONVG = .TRUE.                                            EQLNU117     002046
00774            IF(TT    .LT.TLOW.OR.TT    .GT.THIGH)WRITE(JOUT,306)TT,NPT             002047
01001        306 FORMAT(17H0THE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,I5)EQLNU119  002074
01002            IF(ITNUMB.NE.0) GO TO 160                                              002074
01004            WRITE(JOUT,977) NPT                                                    002076
01007        977 FORMAT (/25X,49H100 ITERATIONS DID NOT SATISFY THE CONVERGENCE REQ     002104
01007           1UIREMENTS FOR POINT,I3/)                                               002104
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01010            IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 873           002104
01012            WRITE(JOUT,874)                                                        002131
01014            TT = T(1)                                                              002136
01015            RETURN                                                                 002140
01015      C     CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.               002140
01016        160 IF(NC.EQ.0) GO TO 143                                                  002144
01020            SIZEF = 0.                                                             002145
01021            INC = 0                                                                002146
01022            DO 170 J = 1,NS                                                        002164
01025            IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-10000) GO TO 170                     002164
01027            INC = INC + 1                                                          002176
01030            IF(RITE)  WRITE(JOUT,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),     002201
01030           1IUSE(J),EN(J,NPT)                                                      002201
01043        144 FORMAT (1H0,3A4,2F10.3,3X,5HIUSE=,I4,E15.7)                            002233
01044            IF (EN(J,NPT))  146,148,169                                            002233
01047        146 IF (J.NE.JSOL .AND. J .NE.JLIQ) GO TO 147                              002236
01051            JSOL = 0                                                               002252
01052            JLIQ = 0                                                               002253
01053        147 IQ1 = IQ1 - 1                                                          002255
01054            EN(J,NPT) = 0.                                                         002257
01055            GO TO 166                                                              002260
01056        148 KG = 1                                                                 002262
01057            IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154                                    002263
01061            IF (J .EQ. 1 .OR. IUSE(J) .NE. -IUSE(J-1))  GO TO 153                  002266
01063            KG = -1                                                                002301
01064        154 JKG = J + KG                                                           002304
01065            IF (EN(JKG,NPT).LT.0.) GO TO 170                                       002306
01067            TMELT = TEMP(INC,1)                                                    002313
01070            IF (TMELT .EQ. TEMP(INC+KG,2))  GO TO 158                              002316
01072            TMELT = TEMP(INC,2)                                                    002322
01073            IF (TMELT .EQ. TEMP(INC+KG,1))  GO TO 157                              002324
01075            WRITE(JOUT,156)                                                        002326
01077        156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER  )        002334
01077      C   JTH SPECIES A SOLID (EN=0), (J+KG)TH SPECIES A LIQUID (EN IS +)          002334
01100       157  IF (TT .GT. TMELT .OR. (TP .AND. TT .EQ. TMELT))  GO TO 169            002334
01102            IF (TP .OR. TT .LE. TMELT - 150.0)  GO TO 1165                         002353
01104            JSOL = J                                                               002365
01105            JLIQ = JKG                                                             002367
01106            GO TO 159                                                              002371
01106      C   JTH SPECIES A LIQUID(EN=0), (J+KG)TH SPECIES A SOLID (EN IS +)           002371
01107       158  IF (TT .LT. TMELT .OR. (TP .AND. TT .EQ. TMELT))  GO TO 169            002373
01111            IF (TP .OR. TT .GE. TMELT + 150.0)  GO TO 1165                         002412
01113            JSOL = JKG                                                             002424
01114            JLIQ = J                                                               002426
01115        159 TLN = ALOG (TMELT)                                                     002431
01116            TT = TMELT                                                             002434
01117            EN(JKG,NPT) = .5 * EN(JKG,NPT)                                         002436
01120            EN(J,NPT) = EN(JKG,NPT)                                                002443
01121            GO TO 165                                                              002444
01121      C   WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN                           002444
01122       1165 EN(J,NPT) = EN (JKG, NPT)                                              002446
01123            IUSE(J) = -IUSE(J)                                                     002451
01124            IUSE (JKG) = -IUSE(JKG)                                                002453
01125            EN(JKG,NPT)= 0.                                                        002456
01126            WRITE(JOUT,161) (SUB(JKG,I), I = 1,3),(SUB(J,I), I = 1,3)              002463
01140       161  FORMAT (1H0,22HPHASE CHANGE, REPLACE ,3A4,6H WITH ,3A4)                002506
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01141            GO TO 40                                                                      002506
01142        153 IF (TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GO TO 169                     002510
01144            IF (TT.GT.TEMP(INC,2)) GO TO 169                                              002525
01146            SUM = 0.                                                                      002534
01147            DO 167 I = 1,L                                                                002543
01152        167 SUM = SUM + A(I,J)*X(I)                                                       002543
01154            DELF = HO(J)-S(J)-SUM                                                         002547
01155            IF(WRITE)  WRITE(JOUT,168)DELF,SIZEF                                          002555
01162        168 FORMAT (17H G0-SUM(AIJ*PI) =E15.7,10X,18HPREVIOUS DELTA G =,E15.7)            002566
01163            IF(DELF.GE.SIZEF .OR. DELF.GE.0.) GO TO 169                                   002566
01165            SIZEF = DELF                                                                  002603
01166            JDELF = J                                                                     002605
01167        169 IF(INC.EQ.NC) GO TO 1160                                                      002610
01171        170 CONTINUE                                                                      002616
01173       1160 IF (SIZEF.EQ.0.) GO TO 143                                                    002616
01175            J = JDELF                                                                     002617
01176        165 IQ1 = IQ1 + 1                                                                 002627
01177            WRITE(JOUT,136) (SUB(J,I), I = 1,3)                                           002624
01205        136 FORMAT (10X,4HADD ,3A4)                                                       002642
01206        166 IUSE(J) = - IUSE(J)                                                           002642
01207         40 CONVG = .FALSE.                                                               002645
01210            JSI = 1                                                                       002645
01211            CALL CPHS                                                                     002647
01212        143 IN = NUMB                                                                     002652
01213            IF (.NOT. SHOCK)  WRITE(JOUT,771) NPT,(X(I), I = 1,L),IN                      002654
01224        771 FORMAT (I3,14F9.3)                                                            002675
01225            JSI = 1                                                                       002675
01226            IF(TP.AND.CONVG)  CALL CPHS                                                   002677
01230            ITNUMB = 100                                                                  002704
01231            GO TO 43                                                   EQLNU126           002706
01231     C      CALCULATE EQUILIBRIUM PROPERTIES                           EQLNU128           002706
01232       1171 DLVPT(NPT) = -1.                                                              002710
01233            DLVTP(NPT) = 1.                                                               002712
01234            CPR(NPT) = CPSUM                                                              002714
01235            GO TO 199                                                                     002715
01236        171 SUM = 0.                                                                      002717
01237            DO 179 J = 1,L                                             EQLNU167           002720
01242        179 SUM = SUM + FROW(J)*X(J)                                                      002733
01244            DLVPT(NPT) = -2.*SUM/ENN+ X(IQ1)                           EQLNU170           002737
01245            IF (JLIQ .EQ. 0)  GO TO 199                                                   002746
01247            IUSE(JLIQ) = -IUSE(JLIQ)                                                      002750
01250            HSUM(NPT) = HSUM(NPT)+EN(JLIQ,NPT)*(HO(JLIQ)-HO(JSOL))                        002753
01251            IQ1 = IQ1+1                                                                   002764
[illegible]      GAMMAS(NPT) = -1./DLVPT(NPT)                                                  002767
[illegible]      GO TO 186                                                                     002772
[illegible]  199 GAMMAS(NPT) = -1./(DLVPT(NPT)+(DLVTP(NPT)**2)*ENN/CPR(NPT))   EQLNU171           002774
[illegible]  186 TTT(NPT) = TT                                              EQLNU178           003005
[illegible]      ENNL = ENL                                                                    003007
01257            PPP(NPT) = PP                                                                 003011
01260            VLM(NPT) = RVR*ENN*TT/PP                                                      003013
01261            HSUM(NPT) = HSUM(NPT)*TT                                                      003020
01262            WM(NPT) = 1./ENN                                           EQLNU180           003023
01263            IF (.NOT. WRITE)  RETURN                                                      003027
[illegible]      WRITE(JOUT,221) NPT,APP(NPT),PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),               003034
[illegible]     1 CPR(NPT),DLVPT(NPT),DLVTP(NPT),GAMMAS(NPT),VLM(NPT)                          003036
[illegible]  221 FORMAT (7H0POINT=I3,3X,4HPCP=E13.6,3X,2HP=E13.6,3X,2HT=E13.6,3X,4H            003052
01303    409*         1H/R=E13.6,3X,4HS/R=E13.6//3X,3HMW=E13.6,3X,5HCP/R=E13.6,3X,6HDLVPT      003057
01303    410*        2=E13.6,3X,6HDLVTP=E13.6,3X,9HGAMMA(S)=E13.6,3X,2HV=,E1' -)              003057
01304    411*          RETURN                                                                  003057
01304    412*   C      ERROR, SET TT=0                                                         003057
01305    413*      673 TT=0.                                                                   003063
01306    414*          NPT = NPT-1                                                             003063
01307    415*          RETURN                                                                  003066
01310    416*          END                                                                     003127
END FOR
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@FOR,S LEWIS.FROZEN,LEWIS.FROZEN
HSA  L5 -10/25/79-17:38:28 (8,)

   SUBROUTINE FROZEN     ENTRY POINT 000345

   STORAGE USED: CODE(1) 000360; DATA(0) 000041; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSTS 000006
    0004    POINTS 000335
    0005    SPECES 012120
    0006    MISC   001264
    0007    INDX   000041

   EXTERNAL REFERENCES (BLOCK, NAME)

    0010    CPHS
    0011    ALOG
    0012    EXP
    0013    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    000066 135G      0001    000251 207G      0001    000022 51L       0001    000050 55L       0001    000120 60L
    0001    000165 81L       0001    000313 901L      0001    000321 903L      0005    006034 A         0006    000570 AM
    0006    000624 AMI       0006    000741 ANUM      0003    000000 ATMN      0006    000004 ATOM      0006    000502 BO
    0006    000521 BOP       0007    000036 CALCH     0000 R  000005 CC        0005    000000 COEF      0007 L  000001 CONVG
    0004 R  000032 CPR       0006    000625 CPRI      0006 R  000564 CPSUM     0006    000604 DATA      0005    005670 DFLN
    0006    001167 DENS      0000 R  000007 DLNT      0004 R  000064 DLVPT     0004 R  000047 DLVTP     0005 R  007734 EN
    0005    005360 ENLN      0006    001263 ENLSAV    0006    000000 ENN       0006    001261 ENNL      0006    001262 ENSAVE
    0006    001073 ENTH      0006    000566 EQRAT     0006    001112 FAZ       0006    001150 FOX       0004 R  000101 GAMMAS
    0003    000001 GMET      0007 L  000003 HP        0006    000572 HPP       0006 R  000567 HSUBO     0004 R  000000 HSUM
    0005 R  005524 HO        0007    000030 IC        0007    000000 IDEBUG    0007    000015 IMAT      0000 I  000010 INC
    0000    000015 INJP$     0007    000023 IONS      0007    000021 IP        0007    000037 IQSAVE    0007    000016 IQ1
    0007    000005 ISV       0007    000034 IT        0005 I  011444 IUSE      0000 I  000004 J         0007    000026 JLIQ
    0007    000025 JSOL      0007 I  000031 JS1       0007    000014 KMAT      0006    000463 LLMT      0007    000040 LSAVE
    0007    000006 MOLES     0006    000626 NAME      0007 I  000024 NC        0007    000022 NEWR      0007 I  000035 NF2
    0007    000012 NLM       0007    000017 NOF       0007    000020 NOMIT     0007    000007 NP        0007 I  000011 NPT
    0007    000027 NREAC     0007 I  000013 NS        0000 I  000000 NSPP1     0007    000010 NT        0006    000565 OF
    0006    001227 OXF       0004    000116 P         0003    000002 PATM      0006    001054 PECWT     0006 R  000563 PP
    0004 R  000117 PPP       0003    000003 RRAR      0003    000004 RRR       0006    000574 RH        0006    001206 RHOP
    0006    001207 RMW       0000 R  000001 RNV       0006    001131 RTEMP     0003 R  000005 RVR       0005 R  002570 S
    0007    000033 SHOCK     0005    011754 SLN       0004    000251 SONVEL    0007 L  000004 SP        0000 R  000006 SS
    0004 R  000015 SSUM      0005    010770 SUB       0000 R  000003 SUMH      0006    000001 SUMN      0000 R  000002 SUMS
    0005 R  000003 SU        0004    000150 T         0005 R  011610 TEMP      0006    000562 THIGH     0006 R  001226 TLN
    0006 R  000560 TLOW      0006    000557 TM        0006    000561 TMID      0004 R  000320 TOTN      0007    000002 TP
    0006 R  [illegible] TT   0004 R  000266 TTT       0004    000202 V         0004 R  000303 VLM       0006    000576 VMIN
    0007 L  000032 VOL       0006    000600 VPLS      0004 R  000234 WM        0006    000602 WP
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00101          SUBROUTINE FROZEN                                                FROZ0002    000000
00101     C                                                                     FROZ0001    000000
00101     C    (FROZEN COMPOSITION EXPANSION ONLY)                              FROZ0004    000000
00101     C                                                                     FROZ0005    000000
00103          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                      /CONSTS/    000000
00104          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                  000000
00104         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)             000000
00104         2 ,VLM(13),TOIN(13)                                                           000000
00104     C    COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)              000000
00104     C   1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)               000000
00105          INCLUDE SPECPK                                                               000000
00111          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),         /MISC/     000000
00111         1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,      /MISC/     000000
00111         2              HSUBO,AM(2),HPP(2) RH(2),VMIN(2),VPLS(2),WP(2),      /MISC/     000000
00111         3              DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),   /MISC/     000000
00111         4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,    /MISC/     000000
00111         5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV               /MISC/     000000
00112          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,   /INDX/     000000
00112         1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,   /INDX/     000000
00112         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE     /INDX/     000000
00112     C                                                                                 000000
00113          LOGICAL CONVG,HP,SP,VOL                                                      000000
00113     C                                                                                 000000
00114          CONVG = .FALSE.                                                              000000
00115          TLN = ALOG(TT)                                                               000000
00116          IF (VOL)  RNV = RVR/(VLM(NPT)*WM(NFZ))                                       000004
00120       51 SUMS=0.                                                                      000022
00121          SUMH = 0.                                                                    000022
00122          JS1 = 1                                                                      000023
00123          J = NPT                                                                      000025
00124          NPT = NFZ                                                                    000027
00125          CALL CPHS                                                                    000031
00126          CC = CPSUM                                                                   000033
00127          IF(.NOT.VOL)  GO TO 55                                                       000035
00131          CC = CPSUM-1./WM(NFZ)                                                        000037
00132          PP = RNV*TT                                                                  000044
00133      55  NPT = J                                                                      000050
00134          DO 60 J = 1,NS                                                               000051
00137          IF (EN(J,NFZ) .LE. 0.0)  GO TO 60                                            000066
00141          SS = S(J)                                                                    000070
00142          IF(IUSE(J).EQ.0)  SS=SS-ALOG(EN(J,NFZ)*PP*WM(NFZ))                           000072
00144          SUMS = SUMS+SS*EN(J,NFZ)                                                     000105
00145          IF (CONVG.OR.HP)  SUMH=SUMH+HO(J)*EN(J,NFZ)                                  000111
00147       60 CONTINUE                                                         FROZ0058    000122
00151          IF (CONVG) GO TO 81                                              FROZ0059    000122
00153          IF(SP)  DLNT=(SUMS-SO)/CC                                                    000124
00155          IF(HP)  DLNT=(SUMH-HSUBO/TT)/CC                                              000132
00157          TLN=TLN-DLNT                                                     FROZ0061    000141
00160          IF(DLNT.LT.0.) DLNT=-DLNT                                                    000144
00162          IF(DLNT.LT.0.5E-4)  CONVG=.TRUE.                                             000151
00164          TT = EXP(TLN)                                                                000157
00165          GO TO 51                                                         FROZ0063    000163
00166       81 TTT(NPT)= TT                                                                 000165
00167          SSUM(NPT)= SUMS                                                              000167
00170          HSUM(NPT)= TT*SUMH                                                           000171
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00171       56*          GAMMAS(NPT)= CPSUM/(CPSUM-1./WM(NFZ))                                      000173
00172       57*          VLM(NPT) = RVR*TT/(WM(NFZ)*PP)                                             000202
00173       58*          WM(NPT) = WM(NFZ)                                                          000210
00174       59*          DLVPT(NPT) = -1.                                                           000212
00175       60*          DLVTP(NPT) = 1.                                                            000214
00176       61*          TOTN(NPT) = TOTN(NFZ)                                                      000215
00177       62*          PPP(NPT) = PP                                                              000217
00200       63*          CPR(NPT)= CPSUM                                                            000221
00201       64*          IF (TT.LT.(TLOW-150.))GO TO 903                                            000223
00203       65*          IF (INC .EQ. 0)  RETURN                                                    000230
00205       66*          INC =0                                                                     000244
00206       67*          DO 901 J = 1,NS                                                            000251
00211       68*          IF (IUSE(J) .EQ. 0 .OR. IUSE(J) .EQ. - 10000)  GO TO 901                   000251
00213       69*          INC = INC+1                                                                000263
00214       70*          IF (EN(J,NFZ) .LE. 0.0)  GO TO 901                                         000267
00216       71*          IF (TT.LT.TEMP(INC,1)-50. .OR. TT.GT.TEMP(INC,2)+50.)  GO TO 903           000272
00220       72*      901 CONTINUE                                                                   000315
00222       73*          RETURN                                                                     000315
00223       74*      903 TT=0.                                                                      000321
00224       75*          NPT= NPT-1                                                                 000321
00225       76*          RETURN                                                                     000324
00226       77*          END                                                   FROZU084             000357
END FOR
```

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@FOR,S LEWIS.GAMEFF,LEWIS.GAMEFF
H A  E3 -10/25/79-17:38:33 (2,)

   SUBROUTINE GAMEFF     ENTRY POINT 000176

   STORAGE USED: CODE(1) 000217; DATA(0) 000044; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003    XPRR
    0004    SQRT
    0005    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   000036 10L       0001   000025 105G       0001   000132 20L       0001   000152 50L       0000 R 000002 ANK
    0000 R 000006 CFA       0000 R 000005 CGAM       0000 R 000001 G         0000 R 000004 GM        0000 R 000003 GP
    0000 I 000000 I         0000   000014 INJP$

00101      1*          SUBROUTINE GAMEFF (V,GAMMAS,A,N,H)                              000025
00103      2*          DIMENSION A(13),GAMMAS(13),H(13),V(13)                          000025
00103      3*     C                                                                    000025
00104      4*          DO 50 I = 2,N                                                   000025
00107      5*          G = GAMMAS(I)                                                   000025
00110      6*          ANK = +1.0                                                      000026
00111      7*          IF (G .GT. 1.0)  GO TO 10                                       000030
00113      8*          G = 1.0010                                                      000033
00114      9*       10 GP = G + 1.0                                                    000036
00115     10*          GM = G - 1.0                                                    000040
00116     11*          CGAM = SQRT(G)*(2.0/GP)**(GP/(2.0*GM))                          000043
00117     12*          CFA = CGAM*SQRT(2.0*G*(1.0 - (1.0/A(I))**(GM/G))/GM)            000063
00120     13*          IF (ABS(V(I) - CFA) .LE. 5.0E-5)  GO TO 50                      000110
00122     14*          IF (G .LT. 2.0)  GO TO 20                                       000115
00124     15*          IF (ANK .LT. 0.0)  GO TO 50                                     000121
00126     16*          ANK = -1.0                                                      000124
00127     17*          G = GAMMAS(I)                                                   000126
00130     18*          GO TO 10                                                        000130
00131     19*       20 G = G + ANK*(V(I) - CFA)                                        000132
00132     20*          IF (G .GT. 1.0)  GO TO 10                                       000136
00134     21*          IF (ANK .LT. 0.0)  GO TO 50                                     000141
00136     22*          ANK = -1.0                                                      000144
00137     23*          G = GAMMAS(I)                                                   000146
00140     24*          GO TO 10                                                        000150
00141     25*       50 H(I) = G                                                        000152
00143     26*          RETURN                                                          000157
00144     27*           END                                                            000216
END FOR
```

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@FOR,S LEWIS.GAUSS,LEWIS.GAUSS
UGA  E_ -10/25/79-17:38:38 (7,)

   SUBROUTINE GAUSS      ENTRY POINT 000411

   STORAGE USED: CODE(1) 000431; DATA(0) 000126; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    DOUBLE 001560
    0004    INDX   000041

   EXTERNAL REFERENCES (BLOCK, NAME)

    0005    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001     000107 10L         0001     000011 110G        0001     000043 120G        0001     000062 127G        0001     000130 152G
    0001     000161 167G        0001     000204 177G        0001     000115 18L         0001     000256 210G        0001     000257 213G
    0001     000141 22L         0001     000361 23L         0001     000333 231G        0001     000167 31L         0001     000275 45L
    0001     000303 47L         0001     000340 51L         0001     000020 8L          0001     000101 9L          0004     000036 CALCH
    0000 D 000000 COEFX       0004     000001 CONVG       0003 D 000000 G           0004     000003 HP          0000 I 000056 I
    0004     000030 IC          0004     000000 IDEBUG      0000     000071 INJP$       0004     000023 IONS        0004     000021 IP
    0004     000037 IOSAVE      0004     000016 IQ1         0004     000005 ISV         0004     000034 IT          0004 I 000015 IUSE
    0000 I 000054 IUSE1       0000 I 000057 J           0004     000026 JLIQ        0004     000025 JSOL        0004     000031 JS1
    0000 I 000061 K           0004     000014 KMAT        0004     000040 LSAVE       0004     000006 MOLES       0004     000024 NC
    0004     000022 NEWR        0004     000035 NFZ         0004     000012 NLM         0000 I 000055 NN          0004     000017 NOF
    0004     000020 NOMIT       0004     000007 NP          0004     000011 NPT         0004     000027 NREAC       0004     000013 NS
    0004     000010 NT          0004     000033 SHOCK       0004     000004 SP          0000 D 000050 SUM         0000 R 000060 TEMP
    0004     000002 TP          0004     000032 VOL         0003 D 001510 X           0000 D 000052 Z


 00101      1*             SUBROUTINE GAUSS                                                                  000000
 00103      2*             COMMON/DOUBLE/G(20,21),X(20)                                                      000000
 00104      3*             COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,     /INDX/         000000
 00104      4*            1              KMAT,IUSE,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,   /INDX/         000000
 00104      5*            2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE    /INDX/         000000
 00105      6*             DOUBLE PRECISION COEFX(20),S,SUM,X,Z                                              000000
 00105      7*      C      BEGIN ELIMINATION OF NNTH VARIABLE                            00205000             003000
 00106      8*             IUSE1=IUSE+1                                                  00203600             000000
 00107      9*             DO 45 NN = 1,IUSE                                                                  000002
 00112     10*             IF (NN .NE. IUSE1)  GO TO 8                                                        000011
 00114     11*             IF (G(NN,NN))  31,23,31                                                            000014
 00114     12*      C      SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW                    00205600             000014
 00117     13*           8 DO 15 I=NN,IUSE                                                                    000020
 00122     14*             COEFX(I) = 1.0E38                                                                  000047
 00123     15*             IF(G(I,NN).EQ.0.)  GO TO 18                                                        000051
 00125     16*             COEFX(I) = 0.                                                                      000054
 00126     17*             DO 16 J=NN,IUSE1                                                                   000062
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00131     18*          SUM = G(I,J)                                                         000062
00132     19*          IF(SUM.LT.0.)  SUM=-SUM                                              000064
00134     20*          IF(J.NE.NN)  GO TO 9                                                 000072
00136     21*          Z = SUM                                                              000075
00137     22*          GO TO 10                                                             000077
00140     23*        9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM                                    000101
00142     24*       10 CONTINUE                                                             000111
00144     25*          COEFX(I) = COEFX(I)/2                                                000111
00145     26*       18 CONTINUE                                                             000121
00147     27*          TEMP = 1.0E38                                                        000121
00150     28*          I=0                                                       00207200   000123
00151     29*          DO 22 J = NN,IUSE                                                    000130
00154     30*          IF (COEFX(J) .GE. TEMP)  GO TO 22                                    000130
00156     31*          TEMP = COEFX(J)                                                      000134
00157     32*          I=J                                                       00207600   000136
00160     33*       22 CONTINUE                                                  00207700   000143
00162     34*          IF (I .EQ. 0)  GO TO 23                                              000143
00162     35*    C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH   00208200   000143
00162     36*    C     VARIABLE FROM THE REMAINING EQUATIONS                         00208300   000143
00162     37*    C      INTERCHANGE EQUATIONS I AND NN                               00208500   000143
00164     38*          IF (NN .EQ. I)  GO TO 31                                             000145
00166     39*          DO 30 J = NN,IUSE1                                                   000150
00171     40*          Z=G(I,J)                                                  00208900   000161
00172     41*          G(I,J)=G(NN,J)                                            00209000   000162
00173     42*      30  G(NN,J) = Z                                                          000164
00173     43*    C     DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH  00209300   000164
00173     44*    C     VARIABLE FROM THE REMAINING EQUATIONS                         00209400   000164
00175     45*       31 K = NN + 1                                                00209600   000167
00176     46*          DO 36 J = K, IUSE1                                        00209700   000171
00201     47*          IF(G(NN,NN).EQ.0.)  GO TO 23                                         000204
00203     48*      36  G(NN,J) = G(NN,J)/G(NN,NN)                                           000207
00205     49*          IF (K .EQ. IUSE1)  GO TO 45                                          000214
00207     50*          DO 44 I = K,IUSE                                                     000217
00212     51*          DO 44 J = K,IUSE1                                                    000257
00215     52*      44  G(I,J) = G(I,J) - G(I,NN)*G(NN,J)                                    000257
00220     53*       45 CONTINUE                                                  00210500   000300
00220     54*    C     BACKSOLVE FOR THE VARIABLES                                   00210700   000300
00222     55*          K = IUSE                                                  00211000   000300
00223     56*       47 J = K + 1                                                 00211100   000303
00224     57*          X(K) = 0.000                                              00203800   000305
00225     58*          SUM = 0.0                                                 00211200   000312
00226     59*          IF (IUSE .LT. J)  GO TO 51                                           000313
00230     60*          DO 50 I = J,IUSE                                                     000316
00233     61*      50  SUM = SUM + G(K,I)*X(I)                                              000333
00235     62*       51 X(K) = G(K,IUSE1) - SUM                                              000340
00236     63*          K = K - 1                                                 00211800   000350
00237     64*          IF (K .NE. 0)  GO TO 47                                              000353
00241     65*          RETURN                                                               000355
00242     66*       23 IUSE = IUSE-1                                                        000361
00243     67*          RETURN                                                               000363
00244     68*          END                                                                  000433
END FOR
```

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@FOR,S LEWIS.HCALC,LEWIS.HCALC
H.A  [illegible] -10/25/79-17:38:44 (9,)

    SUBROUTINE HCALC      ENTRY POINT 000526

    STORAGE USED: CODE(1) 000542; DATA(0) 000066; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003    CONSTS 000006
     0004    HOLCON 000010
     0005    POINTS 000101
     0006    SPECES 011120
     0007    MISC   001264
     0010    INDX   000041
     0011    CCC    000003

    EXTERNAL REFERENCES (BLOCK, NAME)

     0012    CPHS
     0013    ALOG
     0014    NWDU$
     0015    NIO2$
     0016    NERR3$

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001    000070 143G       0001    000107 15L        0001    000131 16L        0001    000145 165G       0001    000154 172G
     0001    000162 177G       0001    000204 210G       0001    000275 227G       0001    000170 30L        0001    000026 4L
     0001    000177 50L        0001    000432 500L       0001    000251 55L        0001    000265 56L        0001    000307 70L
     0001    000427 75L        0000    000010 76F        0001    000477 80L        0000    000024 85F        0001    000037 9L
     0001    000312 90L        0006 R  006034 A          0004 I  000001 AG         0007 R  000570 AM         0007 R  000624 AM1
     0000 R  000002 ANN        0007 R  000741 ANUM       0003    000000 ATMN       0007    000004 ATOM       0004 I  000004 BLK
     0007    000502 BO         0007    000521 BOP        0010 L  000036 CALCH      0006    000000 COEF       0010    000001 CONVG
     0005    000032 CFR        0007 R  000625 CFR1       0007 R  000564 CPSUM      0007 R  000604 DATA       0006    005670 DELN
     0011    000002 DEMAND     0007    001167 DENS       0005    000064 DLVPT      0005    000047 DLVTP      0006 R  002734 EN
     0004    000000 END        0000 R  000007 ENJ        0006    005360 ENLN       0007    001263 ENLSAV     0007    000000 ENN
     0007    001261 ENNL       0007    001262 ENSAVE     0007 R  001073 ENTH       0007    000566 EQRAT      0007 I  001112 FAZ
     0007 I  001150 FOX        0003    000001 GMET       0011    000000 GRAPH      0010    000003 HP         0007 R  000572 HPP
     0007 R  000567 HSUBO      0005    000000 HSUM       0006 R  005524 HO         0000 I  000005 I          0010    000030 IC
     0010    000000 IDEBUG     0004    000002 IE         0010    000015 IMAT       0000    000044 INJP$      0010    000023 IONS
     0010    000021 IP         0010    000037 ICSAVE     0010    000016 IQ1        0000 I  000006 IS         0010    000005 ISV
     0010    000034 IT         0006 I  011444 IUSE       0004 I  000003 IZERO      0010 I  000031 J          0010    000026 JLIO
     0011 I  000001 JOUT       0010    000025 JSOL       0000 I  000004 K          0010    000014 KMAT       0010 I  000012 L
     0007 I  000463 LLMT       0010    000040 LSAVE      0004    000005 MOL        0010 L  000006 MOLES      0000 I  000003 N
     0007 I  000626 NAME       0010    000024 NC         0010    000022 NEWR       0010    000035 NFZ        0010    000017 NOF
     0011    000020 NOMIT      0010    000007 NP         0010 I  000011 NPT        0010 I  000027 NREAC      0010 I  000013 NS
     0000 I  000000 NSPP1      0010    000010 NT         0007 I  000741 NUM        0007 R  000565 OF         0004 I  000006 OX
     0007    001227 OXF        0003    000002 PATM       0007 R  001054 PECWT      0007 R  000563 PP         0003 R  000003 RRAR
     [illegible]               0007    000574 RH         0007    001206 RHOP       0007 R  001207 RMW        0007 R  001131 RTEMP
     [illegible]               0006 R  002570 S          0010 L  000033 SHOCK      0006    011754 SLN        0010    000004 SP
     [illegible]               0006    010770 SUB        0007    000001 SUMN       0007    000003 SO         0006 R  011610 TEMP
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0007 R 000562 THIGH      0007 R 001226 TLN        0007 R 000560 TLOW       0007 R 000557 TM         0007   000561 TMID
0010   000002 IF         0000 R 000001 TSAVE      0007 R 000002 TT         0007   000576 VMIN       0010 L 000032 VOL
0007   000600 VPLS       0007 R 000602 WP         0004   000007 ZERO


00101            SUBROUTINE HCALC                                                           000000
00101      C   CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS                         000000
00103            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                     /CONSTS/   000000
00104            COMMON /HOLCON/ END,AG,IE,IZERO,BLK,MOL,OX,ZERO                 /HOLCON/   000000
00105            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                000000
00105      C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)            000000
00105      C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)             000000
00106            INCLUDE SPECPK                                                             000000
00112            COMMON /MISC/ ENN,SUMN,TT,SD,ATOM(3,101),LLMT(15),BO(15),       /MISC/     000000
00112           1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,   /MISC/     000000
00112           2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),   /MISC/     000000
00112           3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15), /MISC/    000000
00112           4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP, /MISC/     000000
00112           5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV            /MISC/     000000
00113            COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,   /INDX/     000000
00113           1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ, /INDX/    000000
00113           2              NREAC,IC,J,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE    /INDX/     000000
00113      C                                                                                000000
00114               COMMON /CCC/ GRAPH,JOUT,DEMAND                                          000000
00114      C                                                                                000000
00115            DIMENSION NUM(15,5)                                                        000000
00116            EQUIVALENCE (ANUM,NUM)                                                     000000
00117            INTEGER AG,BLK,FAZ,FOX,OX                                                  000000
00120            LOGICAL CALCH,MOLES,SHOCK,VOL                                              000000
00121            TSAVE = TT                                                                 000000
00122            IF (AM(1) .GT. 0.0 .AND. AM(2) .GT. 0.0)  GO TO 4                          000001
00124            AMI= AM(2)                                                                 000015
00125            IF (AM(2) .LE. 0.0)  AMI = AM(1)                                           000017
00127            GO TO 9                                                                    000024
00130          4 AMI=(OF+1.)*AM(1)*AM(2)/(AM(1)+OF*AM(2))                                   000026
00131          9 TM = 0.                                                                    000037
00132            IF(PP.GT.0.) TM = ALOG(PP*AMI)                                             000037
00134            SSUM(NPT) = 0.                                                             000051
00135            HPP(1) = 0.                                                                000053
00136            HPP(2) = 0.                                                                000054
00137            HSUBO = 0.                                                                 000055
00140            CPRI = 0.                                                                  000056
00141            ANN = (1.+OF)                                                              000057
00141      C     LOOP ON REACTANTS. IF OXIDANT, K = 1, IF FUEL, K = 2.                      000057
00142            DO 700 N=1,NREAC                                                           000070
00143            K=2                                                                        000070
00146            IF(FOX(N).EQ.OX)K=1                                                        000072
00150            IF(NAME(N,5).NE.IZERO)  GO TO 90                                           000077
00152            IF(.NOT.CALCH)  GO TO 15                                                   000102
00154            TT = RTEMP(N)                                                              000104
00154      C  15 TT IN RANGE                                                                000104
00155         15 IF (SHOCK)  GO TO 16                                                       000107
00157            IF (TT .LT. TLOW - 100.0 .OR. TT .GT. THIGH + 1000.0)  GO TO 75            000117
00161         16 J = NUM(N,5)                                                               000131
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OF POOR QUALITY

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00162         IF (J.NE.0)  GO TO 90                                          000136
00164         DO 10 J=1,L                                                    000145
00167      10 DATA(J) = 0.0                                                  000145
00171         DO 30 I = 1,4                                                  000154
00174         IF (ANUM(N,I) .LE. 0.0)  GO TO 50                              000154
00176         DO 20 J=1,L                                                    000162
00201      20 IF (LLMT(J) .EQ. NAME(N,I))  GO TO 30                          000162
00204      30 DATA(J) = DATA(J) + ANUM(N,I)                                  000170
00206      50 IS=0                                                           000177
00207         DO 70 J=1,NS                                                   000177
00212         IF(IUSE(J).EQ.0)GO TO 55                                       000204
00214         IS = IS+1                                                      000206
00215         IF(FAZ(N).EQ.AG)GO TO 70                                       000212
00217         IF(TT.GT.TEMP(IS,2).AND.TEMP(IS,2).NE.THIGH)  GO TO 70         000215
00221         IF(TT.LT.TEMP(IS,1).AND.TEMP(IS,1).NE.TLOW)  GO TO 70          000232
00223         GO TO 56                                                       000247
00224      55 IF(FAZ(N).NE.AG.AND.FAZ(N).NE.BLK)  GO TO 70                   000251
00226      56 DO 60 I=1,L                                                    000265
00230      60 IF (A(I,J) .NE. DATA(I))  GO TO 70                             000275
00234         NUM(N,5) = J                                                   000303
00235         GO TO 90                                                       000305
00236      70 CONTINUE                                                       000310
00240         GO TO 80                                                       000310
00241      90 IF (MOLES)       ENJ = PECWT(N)/WP(K)                          000312
00243         IF (.NOT.MOLES)       ENJ = PECWT(N)/RMW(N)                    000325
00245         ENJ = ENJ/ANN                                                  000332
00246         IF(K.EQ.1)  ENJ = ENJ*OF                                       000335
00250         IF(NAME(N,5).NE.IZERO)GO TO 500                                000343
00252         I = NS                                                         000346
00253         NS = J                                                         000350
00254         TLN = ALOG(TT)                                                 000352
00255         IF(.NOT.CALCH)  EN(J,NPT) = ENJ                                000356
00257         CALL CPHS                                                      000363
00260         NS = I                                                         000366
00261         IF (HO(J).GT.-.01 .AND. HO(J).LT..01) HO(J) = 0.               000371
00263         RTEMP(N) = TT                                                  000411
00264         IF(VOL) HO(J)=HO(J)-1.                                         000413
00266         ENTH(N) = RBAR*TT*HO(J)                                        000421
00267         CPR1 = CPR1 + CPSUM                                            000426
00270     500 HSUBO = HSUBO + ENTH(N)*ENJ                                    000432
00271         HPP(K) = HPP(K)+ENTH(N)*ENJ                                    000440
00272     900 SSUM(NPT) = SSUM(NPT) + ENJ*(S(J) - ALOG(ENJ) - TM)            000444
00274         TT = TSAVE                                                     000456
00275         HSUBO = HSUBO/RBAR                                             000460
00276         RETURN                                                         000463
00277      75 WRITE(JOUT,76)                                                 000467
00301      76 FORMAT (//20X,57HREACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA  000473
00301        1IN HCALC/)                                                     000473
00302         RETURN                                                         000473
00303      80 WRITE(JOUT,85) N                                               000477
00306      85 FORMAT (//20X,I2,42HTH REACTANT IS NOT IN THERMO DATA IN HCALC/)   000504
00307         RETURN                                                         000504
00310         END                                                            000541
 D FO
```

```
@FOR,S LEWIS.LTCPHS,LEWIS.LTCPHS
HSA  ES -10/25/79-17:38:51 (2,)

   SUBROUTINE LTCPHS     ENTRY POINT 000205

   STORAGE USED: CODE(1) 000221; DATA(0) 000130; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSTS 000006
    0004    LOWTH  001201

   EXTERNAL REFERENCES (BLOCK, NAME)

    0005    PAGIT
    0006    CHRSIZ
    0007    GOUT
    0010    RDATAI
    0011    RDCHAR
    0012    NUCODS
    0013    RDATAF
    0014    NIO1S
    0015    NIO2S
    0016    NERR3S

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    000006 10L        0000    000072 100F       0001    000025 124G       0001    000045 132G       0001    000111 144G
    0001    000113 147G       0001    000124 156G       0001    000026 20L        0001    000051 30L        0001    000122 46L
    0003    000000 ATMN       0004 R 000361 CPL         0003    000001 GMET       0004 R 000551 HL          0000 I 000066 I
    0004 I 001131 ILSP        0000 I 000024 IMN         0000    000107 INJP$      0000 I 000000 INLTMN      0000 I 000012 ISNMN
    0000 I 000015 ITMPMN      0000 I 000067 J           0000 I 000071 K           0004 I 000000 NLTSP       0000 I 000070 NT
    0003    000002 PATM       0003 R 000003 RBAR        0003    000004 RBR        0000 R 000062 RDUM        0003    000005 RVR
    0004 R 000741 SL          0004 R 000001 SUBLT       0004 R 000171 TL


00101      1*              SUBROUTINE LTCPHS                                                 LTCP  10     000000
00101      2*      C                                                                                      000003
00101      3*      C          PROCESS LOW TEMPERATURE  CP,H,S  (VIA MIPS I/O)                             000000
00101      4*      C                                                                                      000000
00101      5*      C          DIMENSION MIPS OUTPUT ARRAYS                                                000000
00103      6*                 DIMENSION INLTMN(10),ISNMN(3),ITMPMN(7),IMN(5,6),RDUM(4)                    000000
00103      7*      C                                                                                      000007
00104      8*              COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                        /CONSTS/    000000
00105      9*              COMMON /LOWTH/ NLTSP,SUBLT(40,3),TL(40,3),CPL(40,3),HL(40,3),      /LOWTH/     000003
00105     10*            1                SL(40,3),ILSP(40)                                   /LOWTH/     000000
00105     11*      C                                                                                      000000
00105     12*      C          SET DATA FOR MIPS OUTPUT                                                    000000
00106     13*                 DATA INLTMN/24HTYPE THE NUMBER OF LOW T,                                    000000
00106     14*            1     36HEMPERATURE SPECIES TO BE ENTERED    /                                   000000
```

```
00111    15*                DATA ISNMN/18HTYPE SPECIES NAME /                                  000000
00112    16*                DATA ITMPMN/42HTYPE NUMBER OF TEMPERATURES,THIS SPECIES<4/         000000
00114    17*                DATA IMN/36HTYPE  TL,CPL,HL,SL  WHERE -                 ,          000000
00114    18*         1               36H  TL-TEMPERATURE                            ,          000000
00114    19*         2               36H CPL-CONSTANT PRESSURE SPECIFIC HEAT,                  000000
00114    20*         3               36H  HL-ENTHALPY                               ,          000000
00114    21*         4               36H  SL-ENTROPY                                /          000000
00114    22*      C                                                                            000000
00116    23*                NLTSP=0                                                            000000
00117    24*                CALL PAGIT                                                         000000
00120    25*                CALL CHRSIZ(3)                                                     000002
00121    26*        10      CALL GOUT(INLTMN,56)                                               000006
00122    27*                CALL RDATAI(1,NLTSP,$10)                                           000011
00122    28*      C                                                                            000011
00122    29*      C            LOOP FOR EACH SPECIES                                           000011
00123    30*                   DO 60 I=1,NLTSP                                                 000016
00126    31*        20         CALL GOUT(ISNMN,17)                                             000026
00127    32*                   CALL RDCHAR(RDUM,2,-1,$20)                                      000031
00130    33*                   DECODE(100,RDUM) (SUBLT(I,J),J=1,3)                             000037
00136    34*        30         CALL GOUT(ITMPMN,42)                                            000051
00137    35*                   CALL RDATAI(1,NT,$30)                                           000056
00140    36*                   IF(NT.LT.1 .OR. NT.GT.3) GO TO 30                               000064
00142    37*                   ILSP(I)=0                                                       000102
00142    38*      C                                                                            000102
00142    39*      C                  LOOP FOR EACH TEMPERATURE                                 000102
00143    40*                         DO 50 K=1,NT                                              000103
00146    41*                         DO 45 J=1,5                                               000113
00151    42*                         CALL GOUT(IMN(J,1),36)                                    000113
00152    43*        45               CONTINUE                                                  000124
00154    44*        46               CONTINUE                                                  000124
00155    45*                         DO 48 J=1,4                                               000124
00160    46*                         RDUM(J)=0.                                                000124
00161    47*        48               CONTINUE                                                  000125
00163    48*                         CALL RDATAF(4,RDUM,$46)                                   000125
00164    49*                         TL(I,K)=RDUM(1)                                           000132
00165    50*                         CPL(I,K)=RDUM(2)                                          000134
00166    51*                         HL(I,K)=RDUM(3)                                           000136
00167    52*                         SL(I,K)=RDUM(4)                                           000140
00170    53*                         ILSP(I)=ILSP(I)+1                                         000142
00171    54*                         CPL(I,K)=CPL(I,K)/RBAR                                    000145
00172    55*                         HL(I,K)=HL(I,K)/(TL(I,K)*RBAR)                            000147
00173    56*                         SL(I,K)=SL(I,K)/RBAR                                      000152
00174    57*        50               CONTINUE                                                  000163
00174    58*      C                                                                            000163
00174    59*      C            END SPECIES LOOP                                                000163
00176    60*        60         CONTINUE                                                        000163
00176    61*      C                                                                            000163
00200    62*                RETURN                                                             000163
00200    63*      C                                                                            000163
00201    64*       100      FORMAT(8A4)                                                        000220
00201    65*      C                                                                            000220
00202    66*                END                                                                000220
END FOR
```

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@FOR,S LEWIS.MAIN,LEWIS.MAIN
HSA  E3 -10/25/79-17:38:58 (12,)

   MAIN PROGRAM

   STORAGE USED: CODE(1) 001235; DATA(0) 000424; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSTS 000006
    0004    HGLCON 000010
    0005    POINTS 000335
    0006    SPECES 012120
    0007    MISC   001264
    0010    INDX   000041
    0011    PERF   000166
    0012    CCC    000003


   EXTERNAL REFERENCES (BLOCK, NAME)

    0013    RDYES
    0014    MPSINT
    0015    PAGIT
    0016    CHRSIZ
    0017    GOUT
    0020    RDATA1
    0021    REACT
    0022    LTCPHS
    0023    RDCHAR
    0024    NDCOD$
    0025    SEARCH
    0026    THERMP
    0027    DETON
    0030    ROCKET
    0031    SHCK
    0032    MPSTRM
    0033    NINTR$
    0034    NWDU$
    0035    NIO2$
    0036    NERR2$
    0037    NREW$
    0040    NRDU$
    0041    NIO3$
    0042    NIO1$
    0043    NWNL$
    0044    NRNL$
    0045    ALOG
    0046    NSTOP$


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    000006 1L        0000    000271 10F        0001    000406 100L       0001    000211 11L        0001    000576 1305L
    0001    000015 1415      0001    000414 1611L      0000    000300 20F        0001    000064 203L       0001    000441 205L
    0001    000447 206L      0000    000346 207F       0001    000474 208L       0000    000306 21F        0001    000502 210L
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0000     000350 211F      0000     000312 22F       0001     000233 240G      0001     000403 25L       0001     001227 3L
0001     001175 301L      0001     001177 302L      0001     000605 304L      0001     000367 320G      0001     000643 322L
0001     000702 323L      0001     000740 333L      0001     000243 39L       0000     000147 400F      0001     000553 414G
0001     001112 432L      0001     000607 433G      0001     000645 450G      0001     000657 457G      0000     000267 5F
0000     000255 52F       0001     001016 526G      0001     001060 543G      0001     001133 565G      0001     001145 570G
0001     001157 575G      0001     000655 722L      0000     000356 724F      0001     000746 745L      0001     001003 746L
0001     001030 748L      0001     001201 790L      0001     001211 791L      0001     001225 800L      0001     000246 90L
0001     000277 97L       0006 R   006034 A         0011     000150 AEAT      0007     000570 AM        0007     000624 AMI
0007     000741 ANUM      0011     000133 APP       0003 R   000000 ATMN      0007     000004 ATOM      0004 I   000004 BLANK
0007     000502 BO        0007 R   000521 BOP       0010 L   000036 CALCH     0006     000000 COEF      0010     000001 CONVG
0005     000032 CPR       0007     000625 CPRI      0007     000564 CPSUM     0007 I   000604 DATA      0006     005670 DELN
0012     000002 DEMAND    0007     001167 DENS      0000 L   000013 DETN      0005     000064 DLVPI     0005     000047 DLVTP
0006 R   002734 EN        0004 I   000000 END       0006 R   005360 ENLN      0007     001263 ENLSAV    0007 R   000000 ENN
0007 R   001261 ENNL      0007     001262 ENSAVE    0006 I   005670 ENSERT    0007     001073 ENTH      0011 L   000165 EQL
0007 R   000566 EQRAT     0000 L   000014 ERATIO    0000 L   000015 FA        0007     001112 FAZ       0000 L   000026 FIRST
0007     001150 FOR       0000 L   000016 FPCT      0005     000101 GAMMAS    0004     000001 GAS       0003     000001 GMET
0012     000000 GRAPH     0010 L   000003 HP        0007     000572 HPP       0007     000567 HSURU     0005     000000 HSUM
0006     005524 H0        0000 I   000027 I         0010     000030 IC        0000 I   000030 ICARD     0010 I   000000 IDEBUG
0004 I   000002 IE        0010     000015 IMAT      0000     000035 INPT2     0000 I   000003 INSERT    0010 L   000023 IONS
0010     000021 IP        0010     000037 IQSAVE    0010 I   000016 IQI       0000 I   000034 IST       0010     000005 ISV
0010 I   000034 IT        0006 I   011444 IUSE      0004 I   000003 IZ        0000 I   000032 J         0010     000026 JLIQ
0012 I   000001 JOUT      0010     000025 JSOL      0010     000031 JSI       0010     000014 KMAT      0010 I   000012 L
0007 I   000463 LLMT      0010     000040 LSAVE     0000 I   000004 MIT       0007 R   001227 MIX       0000 I   000006 MLOW
0000 L   000017 MMHG      0004     000005 MOL       0010 L   000006 MOLES     0007 I   000626 NAME      0010 I   000024 NC
0000 I   000007 NCO       0010 L   000022 NEWR      0010     000035 NFZ       0000 I   000005 NMLT      0010 I   000017 NOF
0010 I   000020 NOMIT     0010 I   000007 NP        0010     000011 NPT       0010 I   000027 NREAC     0010 I   000013 NS
0000 I   000031 NSERT     0000 I   000000 NSPPI     0000 L   000020 NSUM      0010 I   000010 NT        0007 L   000565 OF
0006 I   005360 OMIT      0004     000006 OX        0007 R   001227 OXF       0007 R   000565 OXFL      0005 R   000116 P
0003 R   000002 PATM      0011     000000 PCP       0007     001054 PECWT     0007     000563 PP        0005     000217 PPP
0000 L   000021 PSIA      0003 R   000003 RBAR      0003     000004 RBR       0000 R   000033 RDUM      0013 L   000000 RDYES
0000 I   000001 REAC      0007     000574 RH        0007 R   001206 RHOP      0000 L   000022 RMT       0007     001207 RMW
0007     001131 RTEMP     0003     000005 RVR       0006     002570 S         0010 L   000033 SHOCK     0006     011754 SLN
0007 R   000003 SO        0005     000251 SONVEL    0010 L   000004 SP        0011     000047 SPIM      0005     000015 SSUM
0006 I   010770 SUB       0011     000101 SUBAR     0007 R   000031 SUMN      0011     000116 SUPAR     0000 L   000023 SV
0007 R   000003 S0        0005 R   000150 T         0006     011610 TEMP      0007 R   000562 THIGH     0000 I   000002 THRM
0007     001226 TLN       0007 R   000560 TLOW      0007     000557 TM        0007 R   000561 TMID      0005     000320 TOTN
0010 L   000002 TP        0007     000002 TT        0005     000266 TTT       0000 L   000024 TV        0000 L   000025 UV
0005 R   000202 V         0011     000064 VACI      0005     000303 VLM       0007 R   000576 VMIN      0011     000032 VMOC
0012 L   000032 VOL       0007 R   000600 VPLS      0005     000234 WM        0007 R   000602 WP        0004     000007 ZERO


00100      1*    C  MAIN PROGRAM                                                                 MAIN0002    000000
00100      2*    C                                                                                           000000
00101      3*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                                  /CONSTS/    000000
00103      4*          COMMON /HOLCON/ END,GAS,IE,IZ,BLANK,MOL,OX,ZERO                              /HOLCON/    000001
00104      5*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPI(13)                              000001
00104      6*        1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                          000001
00104      7*        2 ,VLM(13),TOTN(13)                                                                        000001
00104      8*    C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                          000001
00104      9*    C   1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                            000001
00105     10*          INCLUDE SPECPK                                                                           000001
00111     11*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),                     /MISC/      000001
00111     12*        1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                  /MISC/      000001
00111     13*        2              HSURU,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),                  /MISC/      000001
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00111        3            DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),    /MISC/          000001
00111        4            ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,     /MISC/          000001
00111        5            RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                /MISC/          000001
00112         COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,     /INDX/          000001
00112        1            KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,    /INDX/          000001
00112        2            NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE      /INDX/          000001
00113         COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),       /PERF/          000001
00113        1            SUPAR(13),APP(13),AEAT(13),EQL                        /PERF/          000001
00113      C                                                                                    000001
00114           COMMON /CCC/ GRAPH,JOUT,DEMAND                                                  000001
00115         INTEGER BLANK,DATA,END,ENSERT,OMIT,REAC,SUB,THRM                                  000001
00116         DATA INSERT,MIT,NMLT,REAC,THRM/4HINSE,4HOMIT,4HNAME,4HREAC,4HTHER/                000001
00124         DATA MLOW/4HLOW /     59                  60                                      000001
00126         DIMENSION ENSERT(3,[illegible]),NCD(4),OMIT(3,[illegible])                        000001
00127         EQUIVALENCE (DELN,ENSERT),(ENLN,OMIT),(MIX,OXF),(OF,OXF(1)),(SO,SO)               000001
00130         LOGICAL CALCH,DETN,EQL,ERATIO,FA,FPCT,HP,IONS,MMHG,MOLES,NEWR,                    000001
00130        1        NSUM,OF,PSIA,RKT,SHOCK,SP,SV,TP,TV,UV,VOL                                 000001
00130      C                                                                                    000001
00131           LOGICAL RUYES,FIRST                                                             000001
00131      C                                                                                    000001
00132         REAL MIX(26)                                                                      000001
00132      C                                                                                    000001
00133         NAMELIST /INPT2/ DETN,ERATIO,FA,FPCT,HP,IDEBUG,IONS,MIX,MMHG,NSUM, /INPT2/        000003
00133        1                 OF,P,PSIA,RKT,SO,SHOCK,SO,SP,SV,T,TP,TV,UV,V      /INPT2/        000001
00133      C                                                                                    000001
00134         FIRST=.TRUE.                                                                      000001
00135           CALL MPSINT                                                                     000003
00136       1 WRITE(JOUT,400)                                                                   000006
00140         DO 300 I=1,26                                                                     000015
00143         MIX(I) = 0.0                                                                      000015
00144         P(I)= 0.                                                        ODL   115         000015
00145         T(I)= 0.                                                        ODL   116         000016
00146  300    V(I) = 0.0                                                                        000017
00150         TP = .FALSE.                                                    ODL   123         000021
00151         HP=.FALSE.                                                      ODL   124         000022
00152         TV = .FALSE.                                                                      000023
00153         UV = .FALSE.                                                                      000024
00154         SV = .FALSE.                                                                      000025
00155         RKT = .TRUE.                                                                      000026
00156         SHOCK = .FALSE.                                                 ODL   129         000030
00157         DETN = .FALSE.                                                  ODL   130         000031
00160         MMHG    = .FALSE.                                               ODL   133         000032
00161         PSIA = .TRUE.                                                                     000033
00162         NSUM = .FALSE.                                                                    000035
00163         IONS = .FALSE.                                                                    000036
00164         IDEBUG = 0                                                                        000037
00165         FA = .FALSE.                                                                      000040
00166         OF = .TRUE.                                                                       000041
00167         ERATIO = .FALSE.                                                                  000043
00170         FPCT = .FALSE.                                                                    000044
00171         EQL = .TRUE.                                                    ODL   145         000045
00172         NEWR = .FALSE.                                                  MAIN0022        000047
00173  400    FORMAT(1H1)                                                     MAIN0025        000050
00174           CALL PAGIT                                                                      000050
00175           JOUT=6                                                                          000052
00176           IF(-DYES('TYPE   YES  FOR PRINT TO PRINT FILE',3)) JOUT=3                       000054
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00200     203       CONTINUE                                                                    000064
00201               CALL PAGIT                                                                  000064
00202               CALL CHRSIZ(1)                                                              000065
00203               CALL GOUT('LEWIS CHEMICAL EQUILIBRIUM PROGRAM',34)                          000070
00204               CALL GOUT(' ',1)                                                            000074
00205               CALL GOUT('            MAIN MENU',19)                                       000100
00206               CALL GOUT(' ',1)                                                            000104
00207               CALL GOUT(' 1 - READ THERMODYNAMIC DATA FROM CARDS',39)                     000110
00210               CALL GOUT(' 2 - READ LOW TEMP EXTENSION THERMO DATA',40)                    000114
00211               CALL GOUT(' 3 - SELECT REACTANTS',21)                                       000120
00212               CALL GOUT(' 4 - OMIT SPECIES FROM THERMO DATA',34)                          000124
00213               CALL GOUT(' 5 - INSERT CONDENSED SPECIES',29)                               000130
00214               CALL GOUT(' 6 - BEGIN NAMELIST INPUT',25)                                   000134
00215               CALL GOUT(' RETURN - TERMINATE PROGRAM',27)                                 000140
00216                 ICARD=0                                                                   000144
00217             CALL CHRSIZ(4)                                                                000145
00220               CALL RDATAI(1,ICARD,$203)                                                   000150
00221                IF(ICARD.EQ.0) GO TO 3                                                     000155
00223                IF(ICARD.LT.1 .OR. ICARD.GT.6) GO TO 203                                   000157
00225                GO TO(90,39,11,205,108,210),ICARD                                          000175
00225     C                                                                                     000175
00225     C          CALL SUBROUTINE TO READ REACTANT CARDS                                     000175
00226        11 NSERT = 0                                                     4/23/70           000211
00227           NOMIT = 0                                                                       000211
00230           MOLES = .FALSE.                                               MAIN0041          000212
00231           CALL REACT(FIRST)                                                               000213
00232           IF(L.EQ.0)  WRITE(JOUT,52)                                                      000216
00235        52 FORMAT(24H0ERROR IN REACTANT CARDS)                                             000225
00236           CALCH = .FALSE.                                                                 000225
00237           DO 755 I = 1,NREAC                                                              000233
00242      755  IF (NAME(I,5) .EQ. 12)  CALCH = .TRUE.                                          000233
00245           GO TO 203                                                     MAIN0053          000241
00245     C                                                                                     000241
00245     C     READ LOW TEMPERATURE EXTENSION THERMO DATA                                      000241
00246       39  CALL LTCPHS                                                                     000243
00247           GO TO 203                                                                       000244
00247     C                                                                                     000244
00247     C     READ THERMO DATA FROM CARDS AND STORE ON  TAPE 4                                000244
00250        90 NEWR = .TRUE.                                                                   000246
00251           REWIND 4                                                                        000247
00252               CALL GOUT('ADD THERMO DATA HERE',20)                                        000252
00253           READ(5,5) TLOW,TMID,THIGH                                                       000256
00260         5 FORMAT (3F10.3)                                                                 000266
00261           WRITE (4,5) TLOW,TMID,THIGH                                                     000266
00266      97   READ (5,10) DATA,NCD(1)                                                         000277
00272        10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)                                     000310
00273           IF(DATA(1).EQ.BLANK) DATA(1)=END                                                000310
00275           WRITE (4,10) DATA                                                               000315
00300           IF(DATA(1).EQ.END)  GO TO 203                                                   000325
00302           READ (5,20) (DATA(I), I = 1,5),NCD(2),(DATA(J), J = 6,10),NCD(3),               000330
00302          1            (DATA(I), I = 11,14),NCD(4)                                         000330
00312        20 FORMAT(5E15.8,I5/5E15.8,I5/4E15.8,I20)                                          000354
00313           WRITE (4,21) (DATA(I), I = 1,14)                                                000354
00316        21 FORMAT(5E15.8/5E15.8/4E15.8)                                                    000367
00317           DO 25  I=1,4                                                                    000367
00322           IF(NCD(I).EQ.I)  GO TO 25                                                       000367
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00324             WRITE(JOUT,22) (DATA(J),J=1,3)                                            000372
00327           22 FORMAT(28HOERROR IN ORDER OF CARDS FOR ,3A4)                             000404
00330           25 CONTINUE                                                                 000404
00332             GO TO 97                                                                  000404
00332      C                                                                                000404
00332      C     CHECK INSERT CARDS                                                         000404
00333        108        CONTINUE                                                            000406
00334                   CALL PAGIT                                                          000406
00335                   CALL GOUT('TYPE SPECIES TO INSERT(1 PER LINE)',34)                  000407
00336      181          CONTINUE                                                            000414
00337                   CALL RDCHAR(RDUM,2,-1,$203)                                         000414
00340                   NSERT=NSERT+1                                                       000421
00341                   DECODE(207,RDUM) (ENSERT(I,NSERT), I=1,3)                           000424
00344                   GO TO 181                                                           000437
00344      C                                                                                000437
00344      C      CHECK OMIT CARDS                                                          000437
00345        205        CONTINUE                                                            000441
00346                   CALL PAGIT                                                          000441
00347                   CALL GOUT('TYPE SPECIES TO OMIT FROM THERMO DATA',37)               000442
00350      206          CONTINUE                                                            000447
00351                   CALL RDCHAR(RDUM,2,-1,$208)                                         000447
00352                   NOMIT=NOMIT+1                                                       000454
00353                   DECODE(207,RDUM) (OMIT(I,NOMIT), I=1,3)                             000457
00356      207          FORMAT(3A4)                                                         000472
00357                   GO TO 206                                                           000472
00360         208 CONTINUE                                                      MAINU062    000474
00361             NEWR= .TRUE.                                                              000474
00362             REWIND 4                                                                  000475
00363             GO TO 203                                                     MAINU063    000500
00363      C                                                                                000500
00363      C      BEGIN NAMELIST INPT2                                          MAINU065    000500
00364       210   RHOP = 0.0                                                                000502
00365             SO = 0.0                                                                  000502
00366             SP=.FALSE.                                                    ODE   125   000503
00367             VOL = .FALSE.                                                             000504
00370             NT = 1                                                                    000505
00371                   CALL PAGIT                                                          000507
00372                   IF(RDYES('TYPE YES FOR PRESENT INPT2 NAMELIST',35))                 000511
00372          1        WRITE(6,INPT2)                                                      000511
00376                 WRITE(6,211)                                                          000522
00400      211        FORMAT(' BEGIN NAMELIST INPT2 INPUT')                                 000527
00401             READ(5,INPT2)                                                 MAINU086    000527
00404                   CALL PAGIT                                                          000533
00405             WRITE(JOUT,INPT2)                                                         000535
00410             IF(.NOT.TV.AND..NOT.UV.AND..NOT.SV)  GO TO 304                            000541
00412             VOL = .TRUE.                                                              000546
00413             DO 1304  I=1,26                                                           000553
00416             IF (P(I) .GT. 0.0)  P(I) = 1.0/P(I)                                       000553
00420             IF (V(I) .GT. 0.0)  P(I) = V(I)                                           000561
00422             IF (P(I) .LE. 0.0)  GO TO 1305                                            000566
00424        1304 NP = I                                                                    000571
00426        1305 TP = TV                                                                   000576
00427             HP = UV                                                                   000577
00430             SP = SV                                                                   000601
00431             GO TO 3[illegible]                                                        000603
00432         304 DO 305  I=1,26                                                            000607
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00435   182*         IF (P(I) .LE. 0.0)  GO TO 322                                        000607
00437   183*         NP = I                                                     MAIN0090  000612
00440   184*         IF (MMHG) P(NP) = P(NP)/760.                                         000616
00442   185*         IF (PSIA)  P(NP) = P(NP)/PATM                                        000624
00444   186*    305  IF (NSQM)  P(NP) = P(NP)/ATMN                                        000632
00447   187*     322 DO 307 II = 1,26                                                     000645
00452   188*         IF (T(II) .LE. 0.0)  GO TO 722                                       000645
00454   189*    307  NT = II                                                              000650
00456   190*    722  DO 625 IST = 1,26                                                    000657
00461   191*         IF (MIX(IST) .GT. 0.0)  GO TO 323                                    000657
00463   192*         IF(IST.NE.1) GO TO 745                                               000662
00465   193*         WRITE(JOUT,724)                                                      000665
00467   194*    724  FORMAT (//45X,40HNO INPT2 VALUE GIVEN FOR FA, FPCT, OR OF//)         000672
00470   195*         IF (WP(2) .GT. 0.0)  OXFL = WP(1)/WP(2)                              000672
00472   196*         GO TO 333                                                            000700
00473   197*     323 OXFL  = MIX(IST)                                                     000702
00474   198*         IF(FA) OXFL =1./   MIX(IST)                                          000703
00476   199*         IF(FPCT) OXFL =(100.-   MIX(IST))/   MIX(IST)                        000710
00500   200*         IF(.NOT.ERATIO)  GO TO 333                                           000716
00502   201*         EQRAT = MIX(IST)                                                     000720
00503   202*         IF(EQRAT.EQ.1.)  EQRAT = 1.000005                                    000722
00505   203*         OXFL  = (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))             000727
00506   204*     333 OXF(IST) = OXFL                                                      000740
00507   205*    625  NOF = IST                                                            000741
00511   206*    745  IF (.NOT. IONS .OR. LLMT(L) .EQ. IE)  GO TO 746                      000746
00513   207*         L = L+1                                                              000756
00514   208*         IF(LLMT(L).NE.IE)  NEWR=.TRUE.                                       000761
00516   209*         REWIND 4                                                             000771
00517   210*         LLMT(L) = IE                                                         000774
00520   211*         BOP(L,1) = 0.                                                        000777
00521   212*         BOP(L,2) = 0.                                                        001000
00522   213*         GO TO 748                                                            001001
00523   214*     746 IF(LLMT(L).NE.IE)  GO TO 748                                         001003
00525   215*         DO 747  J=1,NS                                                       001006
00530   216*    747  IF (A(L,J) .NE. 0.0)  IUSE(J) = - 10000                              001016
00533   217*         L = L-1                                                              001024
00534   218*     748 IF(NEWR)  CALL SEARCH                                                001030
00534   219*   C     INITIAL ESTIMATES                                                    001030
00536   220*         SO = SO/REAR                                                         001033
00537   221*         ENN = .1                                                             001036
00540   222*         ENNL = -2.3025851                                                    001040
00541   223*         SUMN = ENN                                                 MAIN0141  001042
00542   224*         DO 432 J=1,NS                                              MAIN0145  001060
00545   225*         IF(IUSE(J).GT.0)  IUSE(J)=-IUSE(J)                                   001060
00547   226*         IF(IUSE(J).EQ.-10000.AND.IONS)  IUSE(J) = 0                          001064
00551   227*         EN(J,1) = 0.                                                         001075
00552   228*         ENLN(J) = 0.                                                         001076
00553   229*         IF (IUSE(J).NE.0)  GO TO 432                                         001077
00555   230*         EN(J,1) = ENN/(NS - NC)                                              001101
00556   231*         ENLN(J) = ALOG(EN(J,1))                                              001103
00557   232*     432 CONTINUE                                                             001113
00561   233*         ICI= L+1                                                             001113
00562   234*         IF (NC.EQ.0.OR.NSERT.EQ.0) GO TO 790                                 001116
00564   235*         DO 302 I=1,NSERT                                                     001126
00567   236*         DO 301 J=1,NS                                                        001145
00572   237*         IF(IUSE(J).EQ.0) GO TO 301                                           001150
```

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00574     238*          DO 299 IST = 1,3                                                        001157
00577     239*     299  IF (SUB(J,IST) .NE. ENSERT(IST,I))  GO TO 301                           001157
00602     240*          IQI= IQI+1                                                              001166
00603     241*          IUSE(J)= -IUSE(J)                                                       001171
00604     242*          GO TO 302                                                               001173
00605     243*      301 CONTINUE                                                                001201
00607     244*      302 CONTINUE                                                                001201
00611     245*     790  IF (.NOT. TP .AND. .NOT. HP .AND. .NOT. SP)  GO TO 791                  001201
00613     246*          CALL THERMP                                                             001205
00614     247*          GO TO 800                                                               001207
00615     248*     791  IF (DETN)  CALL DETON                                                   001211
00617     249*          IF(RKT) CALL ROCKET                                                     001214
00621     250*          IF(SHOCK)  CALL SHCK                                                    001220
00623     251*      800 NSERT = 0                                                               001225
00624     252*          GO TO 1                                                     MAINU152    001225
00625     253*       3       CONTINUE                                                           001227
00626     254*               CALL MPSTRM                                                        001227
00627     255*               STOP                                                               001230
00630     256*          END                                                         MAINU153    001234
END FOR
```

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@FOR,S LEWIS.MATRIX,LEWIS.MATRIX
H,A  ES -10/25/79-17:39:09 (8,)

    SUBROUTINE MATRIX     ENTRY POINT 001063

    STORAGE USED: CODE(1) 001107; DATA(0) 000116; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003    POINTS 000335
     0004    SPECES 012120
     0005    MISC   001264
     0006    DOUBLE 001560
     0007    INDX   000041

    EXTERNAL REFERENCES (BLOCK, NAME)

     0010    NERR3$

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001     000102 124G       0001     000103 127G       0001     000126 140G       0001     000215 154G       0001     000244 161G
     0001     000672 175L       0001     000677 185L       0001     000453 217G       0001     001011 230L       0001     000567 244G
     0001     000606 247G       0001     000623 257G       0001     001026 260L       0001     000757 303G       0001     001023 317G
     0001     000276 55L        0001     000346 59L        0001     000372 62L        0001     000376 64L        0001     000511 65L
     0001     000405 70L        0004 R 006034 A          0005     000570 AM         0005     000624 AM1        0005     000741 ANUM
     0005     000004 ATOM       0005 R 000502 BO         0005     000521 BOP        0007     000036 CALCH      0004     000000 COEF
     0007 L 000001 CONVG      0003     000032 CPR        0005     000625 CPR1       0005 R 000564 CPSUM      0005     000604 DATA
     0004     005670 DELN       0005     001167 DENS       0003     000064 DLVPT      0003     000047 DLVTP      0004 R 002734 EN
     0000 R 000013 ENERGY     0004 R 005360 ENLN       0005     001263 ENLSAV     0005 R 000000 ENN        0005     001261 ENNL
     0005     001262 ENSAVE     0005     001073 ENTH       0005     000566 EQRAT      0000 R 000010 F          0005     001112 FAZ
     0005     001150 FOX        0006 D 000000 G          0003     000101 GAMMAS     0007 L 000003 HP         0005     000572 HPP
     0005 R 000567 HSUBO      0003 R 000000 HSUM       0004 R 005524 HO         0000 I 000003 I          0007     000030 IC
     0007     000000 IDEBUG     0007 I 000015 IMAT       0000     000023 INJP$      0007     000023 IONS       0007     000021 IP
     0007     000037 IOSAVE     0007 I 000016 IQ1        0000 I 000001 IQ2        0000 I 000002 IQ3        0007     000005 ISV
     0007     000034 IT         0004 I 011444 IUSE       0000 I 000007 J          0007     000026 JLIQ       0007     000025 JSOL
     0007     000031 JS1        0000 I 000004 K          0000 I 000006 KK         0007 I 000014 KMAT       0007 I 000012 L
     0005     000463 LLMT       0007     000040 LSAVE      0007     000006 MOLES      0005     000626 NAME       0007     000024 NC
     0007     000002 NEWR       0007     000035 NFZ        0007     000017 NOF        0007     000020 NOMIT      0007     000007 NP
     0007 I 000011 NPT        0007     000027 NREAC      0007 I 000013 NS         0000 I 000000 NSPP1      0007     000010 NT
     0005     000565 OF         0005     001227 OXF        0003     000116 P          0005     001054 PECWT      0005     000563 PP
     0005     000217 PPF        0005     000574 RH         0005     001206 RHOP       0005     001207 RMW        0005     001131 RTEMP
     0004 R 002570 S          0007     000033 SHOCK      0004     011754 SLN        0003     000251 SONVEL     0007 L 000004 SP
     0000 R 000011 SS         0000 R 000005 SSS        0003     000015 SSUM       0004     010770 SUB        0005 R 000001 SUMN
     0005 R 000003 SO         0003     000150 T          0004     011610 TEMP       0000 R 000012 TERM1      0005     000562 THIGH
     0005     001226 TLN        0005     000560 TLOW       0005 R 000557 TM         0005     000561 TM10       0003     000320 TOTN
     0007 L 000002 TP         0005 R 000002 TT         0003     000266 TTT        0003     000202 V          0003     000303 VLM
     0005     000576 VMIN       0007 L 000032 VOL        0005     000600 VPLS       0003     000234 WM         0005     000602 WP
     0006 D 001510 X
```

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00101        SUBROUTINE MATRIX                                                           MATXU001   000030
00101   C                                                                                           000030
00103        COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                            000030
00103       1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                       000030
00103       2 ,VLM(13),TOTN(13)                                                                     000030
00103   C    COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                        000030
00103   C   1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                         000030
00104        INCLUDE SPECPK                                                                         000030
00110        COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,IQ1),LLMT(15),BO(15),                 /MISC/     000030
00110       1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,             /MISC/     000030
00110       2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),             /MISC/     000030
00110       3              DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),          /MISC/     000030
00110       4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,           /MISC/     000030
00110       5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                      /MISC/     000030
00111        COMMON /DOUBLE/ G(20,21), X(20)                                           MATXU012   000030
00112        COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,             /INDX/     000030
00112       1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,          /INDX/     000030
00112       2              NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE            /INDX/     000030
00112   C                                                                                           000030
00113        DOUBLE PRECISION G,X                                                                   000030
00114        LOGICAL CONVG,HP,SP,TP,VOL                                                             000030
00114   C                                                                                           000030
00115        IQ2 = IQ1 + 1                                                                          000030
00116        IQ3 = IQ2 + 1                                                                          000033
00117        KMAT = IQ3                                                                MATXU018   000035
00120        IF(.NOT.CONVG.AND.TP) KMAT = IQ2                                          MATXU019   000036
00122        IMAT = KMAT - 1                                                           MATXU020   000046
00122   C    CLEAR MATRIX STORAGES TO ZERO                                             MATXU022   000046
00123        DO 211 I=1,IMAT                                                                        000057
00126        DO 211 K=1,KMAT                                                                        000103
00131    211 G(I,K) = 0.0D0                                                                         000103
00134        SSS = 0.                                                                               000111
00135        HSUM(NPT) = 0.                                                                         000112
00135   C    BEGIN SET UP OF ITERATION MATRIX                                          MATXU028   000112
00136        KK = L                                                                                 000114
00137        DO 65  J=1,NS                                                             MATXU031   000127
00142        IF(IUSE(J).LT.0)  GO TO 65                                                             000141
00144        IF(IUSE(J).GT.0)  GO TO 70                                                             000145
00146        F = (HO(J)-S(J)+ENLN(J)+TM)*EN(J,NPT)                                                  000150
00147        SS = HO(J)*EN(J,NPT) - F                                                               000157
00150        TERM1 = HO(J)*EN(J,NPT)                                                                000161
00151        IF (KMAT .EQ. IQ2) TERM1 = F                                              MATXU037   000163
00152        DO 55 I = 1, L                                                            MATXU038   000174
00153   C    CALCULATE THE ELEMENTS  R(I,K)                                            MATXU040   000174
00156        IF (A(I,J) .EQ. 0.) GO TO 55                                              MATXU042   000232
00160        DO 15  K=I, L                                                             MATXU044   000234
00163     15 G(I,K) = G(I,K) + A(K,J)*A(I,J)*EN(J,NPT)                                              000244
00165        G(I,IQ1) = G(I,IQ1) + A(I,J)*EN(J,NPT)                                                 000251
00166        G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1                                            MATXU048   000255
00167        IF (CONVG .OR.TP) GO TO 55                                                MATXU049   000261
00171        G(I,IQ3)= G(I,IQ3)+A(I,J)*F                                               MATXU050   000263
00172        IF (SP) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS                                   MATXU051   000267
00174     55 CONTINUE                                                                  MATXU052   000305
00176        IF (KMAT .EQ. IQ2) GO TO 64                                               MATXU053   000305
00200        IF(CONVG.OR.HP) GO TO 59                                                  MATXU054   000310
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00202             G(IQ2,IQ1) = G(IQ2,IQ1) + SS                        MATXU055  000323
00203             G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*SS                      MATXU056  000326
00204             G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - ENLN(J)-TM)*F       MATXU057  000334
00205             GO TO 62                                            MATXU058  000344
00206        59   G(IQ2,IQ2) = G(IQ2,IQ2) + HO(J)**2*EN(J,NPT)                  000346
00207             IF (CONVG) GO TO 64                                 MATXU060  000362
00211             G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*F                       MATXU061  000364
00212        62 G(IQ1,IQ3)=G(IQ1,IQ3)+F                               MATXU062  000372
00213        64 G(IQ1,IQ2)=G(IQ1,IQ2)+TERM1                           MATXU063  000376
00214             GO TO 65                                                      000403
00214     C    CONDENSED SPECIES                                                000403
00215        70 KK = KK + 1                                                     000405
00216             DO 75  I = 1,L                                                000407
00221             G(I,KK) = A(I,J)                                              000453
00222        75   G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)                      000454
00224             G(KK,IQ2) = HO(J)                                             000462
00225             G(KK,KMAT) = HO(J) - S(J)                                     000465
00226             HSUM(NPT) = HSUM(NPT) + HO(J)*EN(J,NPT)                       000471
00227             IF(.NOT.SP) GO TO 65                                          000477
00231             SSS = SSS + S(J)*EN(J,NPT)                                    000501
00232             G(IQ2,KK) = S(J)                                              000505
00233        65 CONTINUE                                              MATXU064  000520
00235             SSS = SSS + G(IQ2,IQ1)                                        000520
00236             HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)                            000527
00237             G(IQ1,IQ1) = SUMN - ENN                                       000537
00237     C       REFLECT SYMMETRIC PORTIONS OF THE MATRIX            MATXU066  000537
00240             K = IQ1                                                       000543
00241             IF (HP .OR. CONVG)  K = IQ2                                   000545
00243             DO 102 I = 1,K                                                000562
00246             DO 102 J = I,K                                                000606
00251       102   G(J,I) = G(I,J)                                               000606
00251     C       COMPLETE THE RIGHT HAND SIDE                        MATXU074  000606
00254             IF(CONVG)  GO TO 175                                MATXU076  000612
00256             DO 145 I=1,L                                        MATXU077  000623
00261             X(I)=BO(I)-G(I,IQ1)                                           000623
00262       145   G(I,KMAT) = G(I,KMAT) + X(I)                                  000625
00264             G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN                  MATXU080  000630
00264     C       COMPLETE ENERGY ROW AND TEMPERATURE COLUMN          MATXU082  000630
00265             IF (KMAT .EQ. IQ2) GO TO 185                        MATXU084  000636
00267             IF (SP)ENERGY = SO+ENN-SUMN - SSS                             000641
00271             IF(HP)ENERGY=HSUBO/TT - HSUM(NPT)                             000656
00273             G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY                                 000665
00274       175 G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM                          MATXU088  000672
00275       185   IF (.NOT. VOL .OR. CONVG)  RETURN                             000677
00275     C       CONSTANT VOLUME MATRIX                                        000677
00277             K = IQ1 - 1                                                   000704
00300             IF(KMAT.EQ.IQ2) GO TO 230                                     000707
00302             DO 220 I = 1,K                                                000721
00305             G(IQ1,I) = G(IQ2,I)-G(IQ1,I)                                  000757
00306             G(I,IQ1) = G(I,IQ2)-G(I,IQ1)                                  000761
00307       220   G(I,IQ2) = G(I,IQ3)                                           000764
00311             G(IQ1,IQ1) = G(IQ2,IQ2)-G(IQ1,IQ2)-G(IQ2,IQ1)                 000767
00312             G(IQ1,IQ2) = G(IQ2,IQ3)-G(IQ1,IQ3)                            000774
00313             IF (HP)  G(IQ1,IQ2) = G(IQ1,IQ2) + ENN                        001001
00315             GO TO 240                                                     001007
00316       230   DO 240 I = 1,K                                                001011
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00321     112*        240  G(I,IQ1) = G(I,IQ2)                                  001023
00323     113*         260 KMAT = IMAT                                          001026
00324     114*             IMAT = IMAT-1                                        001027
00325     115*             RETURN                                               001031
00326     116*             END                                MATXU090          001106
END FOR
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@FOR,S LEWIS.OUT1,LEWIS.OUT1
HSA  E: -10/25/79-17:39:20 (2,)

   SUBROUTINE OUT1        ENTRY POINT 001137
              OUT2        ENTRY POINT 001142
              OUT3        ENTRY POINT 001145

   STORAGE USED: CODE(1) 001150; DATA(0) 000226; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSTS 000006
    0004    HOLCON 000010
    0005    POINTS 000335
    0006    SPECES 012120
    0007    MISC   001264
    0010    INDX   000041
    0011    PERF   000166
    0012    OUP1   000073
    0013    CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0014    VARFMT
    0015    NWDU$
    0016    NI01$
    0017    NI02$
    0020    NI03$
    0021    SQRT
    0022    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000   000103 1F        0001   000034 10L       0001   000025 142G      0001   000043 152G      0001   000625 160L
    0001   000112 166G      0001   000651 170L      0001   000657 175L      0001   000726 177L      0001   000764 179L
    0001   000766 180L      0000   000062 20F       0001   001041 200L      0001   001076 210L      0001   001100 211L
    0001   000175 223G      0001   000205 230G      0000   000037 240F      0001   000233 241G      0001   000256 253G
    0001   000264 260G      0001   000303 270G      0001   000313 276G      0000   000112 280F      0000   000126 290F
    0001   000003 30L       0000   000154 300F      0001   000332 306G      0000   000156 310F      0001   000340 313G
    0000   000122 320F      0001   000356 322G      0001   000402 336G      0000   000116 340F      0001   000423 347G
    0001   000444 360G      0001   000452 365G      0001   000467 374G      0001   000506 404G      0001   000516 412G
    0001   000542 422G      0001   000602 441G      0001   000605 444G      0001   000065 45L       0001   000613 451G
    0001   000636 462G      0001   000645 467G      0001   000201 50L       0001   000664 501G      0001   000723 512G
    0001   000754 524G      0001   001002 546G      0001   001014 551G      0001   001036 560G      0001   001067 572G
    0000   000111 60F       0006   006034 A         0011   000150 AEAT      0007   000570 AM        0007   000624 AM1
    0007 R 000741 ANUM      0011   000133 AFP       0003 R 000000 ATMN      0007   000004 ATOM      0007   000502 BO
    0007   000521 BCF       0010   000036 CALCH     0006   000000 COEF      0010   000001 CONVG     0005 R 000032 CPR
    0007   000625 CPF1      0007   000564 CPSUM     0007   000604 DATA      0006   005670 DELN      0013   000002 DEMAND
    0007 R 001167 DENS      0005 R 000064 DLVPT     0005 R 000047 DLVTP     0006 R 002734 EN        0004   000000 END
    0006   005360 DHLN      0007   001263 ENLSAV    0007   000000 ENN       0007   001261 ENNL      0007   001262 ENSAVE
    0007 R 001073 ENTH      0011 L 000165 ECL       0007 R 000566 EQRAT     0012   000002 FA        0012 R 000003 FAP
    0007 R 001112 FA2       0012 R 000005 FB        0012   000006 FC        0012 R 000007 FCP       0012   000012 FCST
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0012     000014 FCV       0012 R 000015 FG        0012     000017 FGE       0012     000020 FGV       0012 R 000021 FH
0012     000023 FI        0012     000025 FIV       0012 R 000027 FM        0012 R 000031 FMT       0012     000053 FN
0012 R 000052 FOUR      0007 I 001150 FOX       0012     000053 FP        0000 R 000036 FPC       0012 R 000054 FS
0012 R 000056 FSV       0012 R 000057 FT        0012 R 000061 FTK       0012 R 000063 FV        0012 R 000065 FVEL
0000 R 000001 FVLM      0012 R 000001 F13       0012     000000 F9X       0005 R 000101 GAMMAS    0004     000001 GAS
0013     000001 GMET      0013     000000 GRAPH     0000 R 000003 HEAD      0010     000003 HP        0007     000572 HPP
0007     000567 HSUBO     0005 R 000000 HSUM      0006     005524 HO        0000 I 000035 I         0010     000030 IC
0010     000000 IDEBUG    0004     000002 IE        0010     000015 IMAT      0000     000207 INJP$     0010     000023 IONS
0010     000021 IP        0010     000037 IOSAVE    0010     000016 IOI       0010     000005 ISV       0010     000034 IT
0006     011444 IUSE      0004     000003 IZ        0000 I 000034 J         0010     000026 JLIQ      0013 I 000001 JOUT
0010     000025 JSOL      0010     000031 JSI       0000 I 000032 K         0010     000014 KMAT      0004 I 000004 LANK
0007     000463 LLMT      0010     000040 LSAVE     0004     000005 MOL       0010 L 000006 MOLES     0000 I 000014 MW
0007 I 000626 NAME      0010     000024 NC        0000 I 000033 NO        0010     000022 NEWR      0010     000035 NFZ
0010     000012 NLM       0010     000017 NOF       0010     000020 NOMIT     0010     000007 NP        0010 I 000011 NPT
0010 I 000027 NREAC     0010 I 000013 NS        0000 I 000000 NSPP1     0010     000010 NT        0007 R 000565 OF
0012 R 000067 ONE       0004 I 000006 OX        0007     001227 OXF       0005     000116 P         0003     000002 PATM
0011     000000 PCP       0007 R 001054 PECWT     0007     000563 PP        0005 R 000217 PPP       0003 R 000003 RBAR
0003 R 000004 RBR       0007     000574 RH        0007 R 001206 RHOP      0007     001207 RMW       0007 R 001131 RTEMP
0003     000005 RVR       0006     002570 S         0010     000033 SHOCK     0006     011754 SLN       0005 R 000251 SONVEL
0010     000004 SP        0011     000047 SPIM      0005 R 000015 SSUM      0006 R 010770 SUB       0011     000101 SUBAR
0007     000001 SUMN      0011     000116 SUPAR     0007     000003 SD        0005     000150 T         0006     011610 TEMP
0007     000562 THIGH     0012     000070 THREE     0007     001226 TLN       0007     000560 TLOW      0007     000557 TM
0007     000561 TMID      0005 R 000320 TOTN      0010     000002 TP        0007     000002 TT        0005 R 000266 TTT
0012 R 000071 TWO       0005 R 000202 V         0011     000064 VACI      0005 R 000303 VLM       0007     000576 VMIN
0011     000032 VMOC      0010 L 000032 VOL       0007     000600 VPLS      0005 R 000234 WM        0007     000602 WP
0000 R 000020 YN        0000 R 000025 YX        0006 R 005524 Z         0004     000007 ZERO      0012     000072 ZEROF
```

```
00101            SUBROUTINE OUT1                                              OUTPU001    000000
00101        C                                                                            000000
00103            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                  /CONSTS/    000000
00104            COMMON /MOLCON/ END,GAS,IE,IZ,LANK,MOL,OX,ZERO               /MOLCON/    000000
00105            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)              000000
00105           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)         000000
00105           2 ,VLM(13),TOTN(13)                                                       000000
00105        C   COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)          000000
00105        C  1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)           000000
00106            INCLUDE SPECPK                                                           000000
00112            COMMON /MISC/ ENN,SUMN,TT,SD,ATOM(3,101),LLMT(15),BO(15),    /MISC/      000000
00112           1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT, /MISC/     000000
00112           2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2), /MISC/     000000
00112           3              DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15), /MISC/  000000
00112           4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP, /MISC/   000000
00112           5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV          /MISC/     000000
00113            COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS, /INDX/   000000
00113           1              KMAT,IMAT,IQI,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ, /INDX/  000000
00113           2              NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE /INDX/    000000
00114            COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),   /PERF/     000000
00114           1              SUPAR(13),APP(13),AEAT(13),EUL                  /PERF/     000000
00115            COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2), /OUPT/   000000
00115           1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/ 000000
00115           2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE, /OUPT/  000000
00115           3              TWO,ZEROF                                       /OUPT/     000000
00115        C                                                                            000000
```

```
00116             COMMON /CCC/GRAPH,JOUT,DEMAND                                          000000
00116       C                                                                            000000
00117             DIMENSION FVLM(2),HEAD(9),MW(2,2),YN(5),YX(5),Z(10,3)                   000000
00120             EQUIVALENCE (Z,HO)                                                     000000
00121             INTEGER FOX,OX                                                         000000
00122             LOGICAL EQL,MOLES,VOL                                                  000000
00122       C                                                           OUTPU021         000000
00122       C     HEAD = (1XA6,2X5(A2,F8.5,3X), 5X,F7.5,F13.3,4X,A1,F10.2,F9.4)           000000
00122       C                                                                            000000
00123             DATA HEAD/6H(1XA6,,6H2X5(A2,6H,F8.4,,6H3X), 5,6HX,F7.5,6H,F13.3,        000000
00123            1     6H,4X,A1,6H,F10.2,6H,F9.4)/,YN/6H2X1(A2,6H2X2(A2,6H2X3(A2,         000000
00123            2     6H2X4(A2,6H2X5(A2/,YX/6H3X),57,6H3X),44,6H3X),31,6H3X),18,         000000
00123            3 6H3X), 57,MW/24HWT FRACTION    MOLES     /,FVLM/12HVOLUME CC/G /       000000
00123       C                                                                            000000
00131             K = 1                                                                  000000
00132             IF (MOLES)  K = 2                                                      000001
00134             WRITE(JOUT,240) MW(1,K),MW(2,K)                                        000005
00140         240 FORMAT (77X,2A6,34H ENTHALPY   STATE   TEMP   DENSITY/10X,             000025
00146            1        16HCHEMICAL FORMULA,65X,7HCAL/MOL,10X,6HDEG. K,3X,5HG/CM3)       000025
00141             DO 60 K = 1,NREAC                                                      000025
00144             IF (FOX(K) .NE. OX)  GO TO 10                                          000025
00146             ND = 6HOXIDNT                                                          000030
00147             GO TO 30                                              OUT1 580         000032
00150          10 ND = 6HFUEL                                                            000034
00151         30  DO 40 J=1,5                                           OUT1 610         000036
00154          40 IF(ANUM(K,J) .LE. 0. .OR. NAME(K,J) .EQ. LANK)  GO TO 45               000043
00157             J=6                                                                    000062
00160          45 J=J-1                                                                  000065
00161             HEAD(2) = YN(J)                                                        000073
00162             HEAD(4) = YX(J)                                                        000075
00163          60 WRITE(JOUT,HEAD) ND,(NAME(K,I),ANUM(K,I),I = 1,J),PECWT(K),            000077
00163            1                ENTH(K),FAZ(K),RTEMP(K),DENS(K)                        000077
00201             FPC = 100./(1.+OF)                                                     000126
00202             WRITE(JOUT,20)   OF   ,FPC,EQRAT,RHOP                                  000133
00210          20 FORMAT (1H0,15X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,             000144
00210            1  19HEQUIVALENCE RATIO= ,F7.4,4X,8HDENSITY=,F8.4//)                    000144
00211             RETURN                                                                 000144
00211       C                                                                            000144
00212             ENTRY OUT2                                                             000147
00212       C     VOLUME                                                                 000147
00213             FMT(3) = ONE                                                           000147
00214             IF(.NOT.VOL)  GO TO 50                                                 000151
00216             CALL VARFMT(VLM,NPT)                                                   000153
00217             WRITE(JOUT,FMT) FVLM,FB,(VLM(I), I = 1,NPT)                            000157
00217       C   PRESSURE                                                OUTPU038         000157
00227          50 DO 55 I = 1,NPT                                                        000201
00232          55 V(I) = ATMN*PPP(I)                                                     000205
00234             CALL VARFMT(V,NPT)                                                     000213
00235             WRITE(JOUT,FMT) FAP,FB,(V(J), J = 1,NPT)                               000214
00235       C   TEMPERATURE                                             OUTPU047         000214
00245             FMT(3) = F13                                                           000236
00246             FMT(4) = 1.0                                                           000240
00247             WRITE(JOUT,FMT) FTK,FB,(TT(J), J = 1,NPT)                              000242
00247       C   ENTHALPY                                                OUTPU056         000242
00257             DO 75 I=1,NPT                                         OUTPU058         000264
00262          75 V(I) = FBAR*PSUM(I)                                                    000264
```

```
00264            WRITE(JOUT,FMT) FH,FB,(V(J), J = 1,NPT)                                000267
00264      C   ENTROPY                                                      OUTPU064    000267
00274            FMT(4) = FOUR                                                          000306
00275            DO 76 I = 1,NPT                                                        000313
00300       76   V(I) = RBAR*SSUM(I)                                                    000313
00302            WRITE(JOUT,FMT) FS,FB,(V(J), J = 1,NPT)                                000316
00302      C     DENSITY                                                                000316
00312            DO 70 I = 1,NPT                                                        000340
00315       70   IF (VLM(I) .GT. 0.0)  V(I) = 1.0/VLM(I)                                000340
00320            WRITE(JOUT,1) (V(J), J = 1,NPT)                                        000347
00326        1   FORMAT (1X,14HDENSITY G/CC  ,1P13E9.3)                                 000361
00327            WRITE(JOUT,80)                                                         000361
00331       80 FORMAT ( 1H )                                                OUTPU070    000366
00331      C   MOLECULAR WEIGHT                                             OUTPU072    000366
00332            WRITE(JOUT,FMT) FM,FB,(WM(J), J = 1,NPT)                               000366
00332      C   (DLV/DLP)T                                                   OUTPU078    000366
00342            IF (EQL)  WRITE(JOUT,FMT) FT,FB,(DLVPT(J), J = 1,NPT)                  000405
00342      C   (DLV/DLT)P                                                   OUTPU083    000405
00353            IF (EQL)  WRITE(JOUT,FMT) FV,FB,(DLVTP(J), J = 1,NPT)                  000426
00353      C   HEAT CAPACITY                                                OUTPU087    000426
00354            DO 85  I=1,NPT                                             OUTPU089    000452
00367       85   V(I) = RBAR*CPR(I)                                                     000452
00371            WRITE(JOUT,FMT) FCP,(V(J), J = 1,NPT)                                  000455
00371      C   GAMMA(S)                                                     OUTPU093    000455
00400            WRITE(JOUT,FMT) FG,FB,(GAMMAS(J), J = 1,NPT)                           000472
00400      C   SONIC VELOCITY                                               OUTPU097    000472
00410            FMT(4) = TWO                                                           000511
00411            DO 95 I = 1,NPT                                            OUTPU100    000516
00414       95   SONVEL(I) = SQRT(RBR*GAMMAS(I)*TTT(I)/WM(I))                           000516
00416            WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(J), J = 1,NPT)                        000527
00426            RETURN                                                                 000545
00426      C                                                                OUTP0104    000545
00427            ENTRY OUT3                                                             000550
00430            WRITE(JOUT,80)                                                         000550
00432            ND = 0                                                                 000555
00432      C     MOLE FRACTIONS EQUILIBRIUM OR FROZEN                       OUT12270    000555
00433            WRITE(JOUT,280)                                                        000556
00435      280   FORMAT (15H0MOLE FRACTIONS/)                                           000563
00436            IF (.NOT. EQL)  GO TO 175                                              000563
00436      C     EQUILBRIUM MOLE FRACTIONS                                              000563
00440            DO 170 K=1,NS                                              OUT12330    000605
00443            DO 140 I=1,NPT                                             OUT12340    000605
00444       140  V(I) = EN(K,I)/TOTN(I)                                                 000605
00450            DO 150 I=1,NPT                                             OUT12370    000613
00453       150  IF (V(I) .GE. 5.0E-7)  GO TO 160                                       000613
00456            ND = 1                                                                 000621
00457            GO TO 170                                                  OUT12400    000623
00463       160  WRITE(JOUT,340) (SUB(K,J), J = 1,3),FB,(V(I), I = 1,NPT)               000625
00473       340  FORMAT (1H ,3A4,A2,1P13E9.3)                                           000655
00474       170  CONTINUE                                                   OUT12430    000655
00474      C     OUTPUT COMPLETE GO EXIT                                    OUT12590    000655
00476            GO TO 11                                                   OUT12600    000655
00476      C     FROZEN MOLE FRACTIONS                                                  000655
00477       175  J = 0                                                                  000657
00500            DO 179 K = 1,NS                                            OUT12630    000657
00503            V(J+1) = EN(K,1)/TOTN(1)                                               000671
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ORIGINAL PAGE IS
OF POOR QUALITY

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00504     139*          IF (V(J+1) .LT. 5.0E-7)  ND = 1                                       000675
00506     140*          IF (V(J+1) .LT. 5.0E-7)  GO TO 177                                    000704
00506     141*    C     OUTPUT VALUE ACCEPTED                                      OUT12660   000704
00510     142*          J = J + 1                                                             000711
00511     143*          DO 176 I = 1,3                                                        000714
00514     144*     176  Z(J,I) = SUB(K,I)                                                     000723
00516     145*     177  IF (J .NE. 4 .AND. K .NE. NS)  GO TO 179                              000726
00520     146*          IF (J .EQ. 0)  GO TO 180                                              000741
00522     147*          WRITE(JOUT,320) (Z(I,1),Z(I,2),Z(I,3),V(I), I = 1,J)                  000743
00533     148*     320  FORMAT (1H ,4(3A4,F11.8,5X))                                          000762
00534     149*          J = 0                                                                 000762
00535     150*     179  CONTINUE                                                   OUT12750   000766
00537     151*     180  IF (ND .EQ. 0)  GO TO 211                                             000765
00541     152*          WRITE(JOUT,290)                                                       000767
00543     153*     290  FORMAT (//1X,116HADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHO    000774
00543     154*         1SE MOLE FRACTIONS WERE LESS THAN 5.0E-7 FOR ALL ASSIGNED CONDITION    000774
00543     155*         2S//)                                                                  000774
00544     156*          J = 0                                                                 000774
00545     157*          DO 210 K=1,NS                                              OUT12780   001002
00550     158*          DO 190 I=1,NPT                                             OUT12790   001014
00553     159*     190  IF( (EN(K,I)/TOTN(I)) .GE. (5.0E-7) ) GO TO 200            OUT12800   001014
00556     160*          J = J + 1                                                             001024
00557     161*          DO 195 I = 1,3                                                        001027
00562     162*     195  Z(J,I) = SUB(K,I)                                                     001036
00564     163*     200  IF (J .NE. 10 .AND. K .NE. NS)  GO TO 210                             001041
00566     164*          IF (J .EQ. 0)  GO TO 211                                              001054
00570     165*          WRITE(JOUT,300) (Z(I,1),Z(I,2),Z(I,3), I = 1,J)                       001056
00600     166*    300   FORMAT (10(1X,3A4))                                        OUT13100   001074
00601     167*          J = 0                                                                 001074
00602     168*    210   CONTINUE                                                   OUT12900   001100
00604     169*     211  IF (.NOT. MOLES)  WRITE(JOUT,310)                                     001100
00607     170*     310  FORMAT (//1X,77HNOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND O    001106
00607     171*         1F OXIDANT IN TOTAL OXIDANTS)                                          001106
00610     172*          RETURN                                                                001106
00611     173*          END                                                        OUTPU137   001147
END FOR
```

```
@FOR,S LEWIS.REACT,LEWIS.REACT
HSA  LS -10/25/79-17:39:27 (11,)

   SUBROUTINE REACT      ENTRY POINT 000714

   STORAGE USED: CODE(1) 000730; DATA(0) 000167; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    MOLCON 000010
    0004    MISC   001264
    0005    INDX   000041
    0006    CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0007    FREAD
    0010    NRLW$
    0011    NRDU$
    0012    NI02$
    0013    NIO1$
    0014    NWDU$
    0015    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000     000107 10F       0001     000256 101L      0001     000003 121G      0001     000013 132G      0001     000053 154G
    0001     000104 177G      0001     000040 20L       0001     000355 200L      0000     000110 21F       0001     000414 210L
    0001     000551 218L      0001     000553 220L      0001     000615 222L      0001     000620 224L      0001     000635 226L
    0001     000657 229L      0001     000342 230G      0001     000673 230L      0001     000172 236G      0001     000205 245G
    0001     000227 260G      0001     000326 303G      0000     000123 31F       0001     000371 321G      0001     000411 335G
    0001     000432 344G      0001     000475 355G      0001     000155 37L       0001     000525 370G      0001     000601 405G
    0001     000604 410G      0001     000625 426G      0001     000650 441G      0001     000217 45L       0001     000663 450G
    0001     000224 46L       0001     000240 50L       0004 R   000570 AM        0004     000624 AM1       0004 R   000626 ANAME
    0004 R   000741 ANUM      0004 R   000004 ATOM      0004     000502 BO        0004 R   000521 BOP       0005     000036 CALCH
    0005     000001 CONVG     0004     000625 CPR1      0004     000564 CPSUM     0004 R   000604 DATA      0006     000002 DEMAND
    0004 R   001167 DENS      0003     000000 END       0004     001263 ENLSAV    0004     000000 ENN       0004     001261 ENNL
    0004     001262 ENSAVE    0004 R   001073 ENTH      0004     000566 EQRAT     0004 R   001112 FAZ       0004 I   001150 FOX
    0005     000001 GAS       0006     000000 GRAPH     0005     000003 HP        0004 R   000572 HPP       0004     000567 HSUB0
    0000 I   000102 I         0005     000030 IC        0005     000000 IDEBUG    0003     000002 IE        0005     000015 IMAT
    0000     000144 INJP$     0000 I   000075 IO        0005     000023 IONS      0005     000021 IP        0005     000037 IQSAVE
    0005     000016 IQ1       0005     000005 ISV       0005     000034 IT        0003 I   000003 IZERO     0000 I   000077 J
    0000 I   000105 JJ        0005     000026 JLIQ      0006 I   000001 JOUT      0005     000025 JSOL      0005     000031 JS1
    0000 I   000076 K         0005     000014 KMAT      0005 I   000012 L         0003 I   000004 LANK      0004 I   000463 LLMT
    0000 I   000020 LLMTS     0005     000040 LSAVE     0003 I   000005 MOL       0000 I   000103 MOLE      0005 L   000006 MOLES
    0000 I   000101 N         0004 I   000626 NAME      0005     000026 NC        0005 L   000022 NEWR      0000 I   000100 NFUEL
    0005     000035 NF2       0000 I   000000 NLS       0005     000017 NOF       0005 I   000020 NOMIT     0005     000007 NP
    0005     000011 NP1       0005 I   000027 NREAC     0005     000013 NS        0005     000010 NT        0004     000565 OF
    0000 I   000006 OV        0004     001227 OXF       0000 R   000106 PCWT      0004 R   001054 PECWT     0004     000563 PP
    0004 R   000574 RH        0004     001206 RHOP      0000 R   000104 RM        0004 R   001207 RMW       0004 R   001131 RTEMP
    0004 R   000037 SHUP      0005     000033 SHOCK     0005     000004 SP        0004     000001 SUMN      0004     000003 SO
    0004     000562 THIGH     0004     001226 TLN       0004     000560 TLOW      0004     000557 TM        0004     000561 TMID
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0005   000002 TP        0004   000002 TT        0000 R 000001 V        0004 R 000576 VMIN      0005   000032 VOL
0004 R 000600 VPLS      0004 R 000602 WP        0003 I 000007 ZERO



00101            SUBROUTINE REACT(FIRST)                                                                  000003
00101      C                                                                                              000003
00103            COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                              /HOLCON/  000003
00104            COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),                      /MISC/    000003
00104           1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                  /MISC/    000003
00104           2              HSUB0,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),                  /MISC/    000003
00104           3              DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),              /MISC/    000003
00104           4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,                /MISC/    000003
00104           5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                           /MISC/    000003
00105            COMMON /INDX/ IDLBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,                  /INDX/    000003
00105           1              KMAT,IMAT,IOI,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,               /INDX/    000003
00105           2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE                 /INDX/    000003
00105      C                                                                                              000003
00106               COMMON /CCC/ GRAPH,JOUT,DEMAND                                                        000003
00106      C                                                                                              000003
00107            DATA NLS/0/                                                                              000003
00111            DIMENSION ANAME(15,5),V(15),LLMTS(15),SBUP(15,2)                                         000003
00112            EQUIVALENCE (NAME,ANAME)                                                                 000003
00113            INTEGER FOX,OX,ZERO                                                                      000003
00114            LOGICAL MOLES,NEWR                                                                       000003
00114      C                                                                                              000003
00115               LOGICAL FIRST                                                                         000003
00116               DATA IO/8/                                                                            000003
00116      C                                                                            RCINU022          000003
00120            DO 8 K = 1,2                                                                             000003
00123            WP(K)=0.                                                                                 000003
00124            HPP(K)=0.                                                                                000003
00125            RH(K)=0.                                                                                 000004
00126            VPLS(K)=0.                                                                               000005
00127            VMIN(K)=0.                                                                               000006
00130            AM(K)=0.                                                                                 000007
00131            DO 8 J=1,15                                                                              000013
00134            LLMT(J)=0                                                                                000013
00135        8   BOP(J,K) = 0.0                                                                           000013
00140            NFUEL = 0                                                                                000017
00141            N=1                                                                                      000020
00142            L=1                                                                                      000022
00142      C                                                                                              000022
00142      C        CALL SUBROUTINE TO SET UP REACTANTS ON FILE 8                                         000022
00143               CALL RREAD(FIRST)                                                                     000023
00143      C                                                                                              000023
00143      C        READ REACTANTS FROM FILE 8                                                            000023
00144               REWIND IO                                                                             000026
00145               READ(IO,10) NREAC                                                                     000031
00150       10   FORMAT(I3)                                                                               000040
00150      C                                                                                              000040
00151       20      CONTINUE                                                                              000040
00152            READ(8,21)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ(N)                       000040
00152           1 ,RTEMP(N),FOX(N),DENS(N)                                                                000040
00170       21      FORMAT(2X,5(A2,F8.4,2X),/,F10.6,2X,A1,F13.4,4X,A1,F12.3,                              000067
00170          1   3X,A1,F12.5,1X)                                                      000067
00171            IF(NAME(N,1).EQ.LANK) GO TO 200                                         000067
00173            IF(L.EQ.0)GO TO 20                                                      000072
00175            WRITE(JOUT,31)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),        000074
00175          1   FAZ(N),FTEMP(N),FOX(N),DENS(N)                                        000074
00213       31   FORMAT(1X,5(A2,F8.4,2X),F10.6,2X,A1,F11.4,2X,A1,F10.3,2X,A1,F11.5)      000121
00214            IF (MOLE .EQ. MOL)  MOLES = .TRUE.                                      000121
00214     C      IF OXIDANT, K = 1; IF FUEL, K = 2.                                      000121
00216            IF(FOX(N).EQ.ZERO)  FOX(N)=OX                                           000126
00220            IF (PECWT(N) .LE. 0.0)  PECWT(N) = 1.0                                  000134
00222            K = 1                                                                   000142
00223            IF(FOX(N).EQ.OX)  GO TO 37                                              000144
00225            K = 2                                                                   000150
00226            NFUEL = NFUEL+1                                                         000152
00227       37 DO 38  J=1,15                                                             000155
00232       38   DATA(J) = 0.0                                                           000162
00234            RM=0.                                                                   000163
00235            DO 100 JJ=1,5                                                           000172
00240            IF (ANUM(N,JJ) .LE. 0.0)  GO TO 101                                     000172
00242            IF (NAME(N,JJ) .EQ. ZERO)  NAME(N,JJ) = OX                              000175
00244            DO 41 J=1,15                                                            000205
00247            I = J                                                                   000205
00250            IF(LLMT(J).EQ.0) GO TO 45                                               000207
00252       41   IF (NAME(N,JJ) .EQ. LLMT(J))  GO TO 46                                  000211
00255       45   L = 1                                                                   000217
00256            LLMT(J)=NAME(N,JJ)                                                      000221
00257       46   DO 48 I = 1,101                                                         000227
00262       48   IF (ATOM(1,I) .EQ. ANAME(N,JJ))  GO TO 50                               000227
00265            L=0                                                                     000235
00266            GO TO 20                                                                000236
00267       50   RM = RM + ANUM(N,JJ)*ATOM(2,I)                                          000240
00270            V(J) = ATOM(3,I)                                                        000246
00271      100   DATA(J) = ANUM(N,JJ)                                                    000250
00273      101 PCWT=PECWT(N)                                                             000256
00274            IF(MOLES) PCWT=PCWT*RM                                                  000261
00276            WP(K)=WP(K) + PCWT                                                      000266
00277            IF (NAME(N,5) .NE. IZERO)  HPP(K) = HPP(K) + ENTH(N)*PCWT/RM            000272
00301            AM(K)=AM(K)+PCWT/RM                                                     000314
00302            DO 110  J=1,L                                                           000326
00305      110   BOP(J,K) = DATA(J)*PCWT/RM + BOP(J,K)                                   000326
00307            IF (DENS(N) .GT. 0.0)  RH(K) = RH(K) + PCWT/DENS(N)                     000333
00311            RMW(N) = RM                                                             000344
00312            N = N+1                                                                 000347
00313            IF(N.NE.16) GO TO 20                                                    000352
00315      200 NREAC =N-1                                                                000355
00316            IF(NFUEL.GT.0)  GO TO 210                                               000357
00316     C      100 PERCENT OXIDANT, CALL REACTANTS FUEL                                000357
00320            DO 205  N=1,NREAC                                                       000371
00323      205   FOX(N) = LANK                                                           000371
00325            RH(2) = RH(1)                                                           000373
00326            RH(1) = 0.                                                              000375
 0327            WP(2) = WP(1)                                                           000376
00330            WP(1) = 0.                                                              000400
00331            HPP(2) = HPP(1)                                                         000401
00332            AM(2) = AM(1)                                                           000403
00333            AM(1) = 0.                                                              000405
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00334            DO 208  J=1,L                                                   000411
00337       208  BOP(J,2) = BOP(J,1)                                             000411
00341       210  IF (L .EQ. 0)  RETURN                                           000414
00343            DO 220 K=1,2                                                    000420
00346            IF (WP(K) .LE. 0.0)  GO TO 220                                  000452
00350            HPP(K)=HPP(K)/WP(K)                                             000455
00351            AM(K) = WP(K)/AM(K)                                             000460
00352            IF (RH(K) .GT. 0.0)  RH(K) = WP(K)/RH(K)                        000463
00354            DO 215 J=1,L                                                    000475
00357            BOP(J,K)=BOP(J,K)/WP(K)                                         000475
00360            IF(V(J).LT.0.)VMIN(K)= VMIN(K)+BOP(J,K)*V(J)                    000477
00362       215  IF (V(J) .GT. 0.0)  VPLS(K) = VPLS(K) + BOP(J,K)*V(J)           000506
00365            IF(MOLES) GO TO 220                                             000520
00367            DO 218 N=1,NREAC                                                000525
00372            IF((FOX(N).EQ.OX.AND.K.EQ.2).OR.(FOX(N).NE.OX.AND.K.EQ.1))GOTO218
                                                                                 000525
00374            PECWT(N) = PECWT(N)/WP(K)                                       000545
00375        218 CONTINUE                                                        000555
00377        220 CONTINUE                                                        000555
00401            NEWR=.TRUE.                                                     000555
00401     C  ARE ELEMENTS SAME AS FOR  LAST SET OF REACTANTS, IF SO, NEWR=.FALSE.  4/23/70   000555
00402            IF (L .NE. NLS .OR. NOMIT .NE. 0)  GO TO 226                    000557
00404            DO 224 I=1,NLS                                                  000571
00407            DO 222 J = 1,L                                                  000604
00412            IF(LLMT(J).NE.LLMTS(I))  GO TO 222                              000604
00414            SBOP(I,1) = BOP(J,1)                                            000607
00415            SBOP(I,2) = BOP(J,2)                                            000611
00416            GO TO 224                                                       000613
00417        222 CONTINUE                                                        000616
00421            GO TO 226                                                       000616
00422        224 CONTINUE                                                        000621
00424            NEWR = .FALSE.                                                  000621
00425            DO 225 I = 1,L                                                  000625
00430            LLMT(I) = LLMTS(I)                                              000625
00431            BOP(I,1)  = SBOP(I,1)                                           000626
00432       225  BOP(I,2) = SBOP(I,2)                                            000630
00434            GO TO 229                                                       000633
00435       226  NLS = L                                                         000635
00436            NOMIT = 0                                          4/23/70      000636
00437            REWIND 4                                                        000641
00440            DO 228 I = 1,L                                                  000650
00443            SBOP(I,1) = BOP(I,1)                                            000650
00444            SBOP(I,2) = BOP(I,2)                                            000651
00445       228  LLMTS(I) = LLMT(I)                                              000653
00447        229 DO 230  N=1,NREAC                                               000657
00452            IF (DENS(N) .GT. 0.0)  GO TO 230                                000663
00454            RH(2) = 0.                                                      000665
00455            RH (1) = 0.                                                     000666
00456            RETURN                                                          000667
00457        230 CONTINUE                                                        000674
00461            RETURN                                                          000674
00462            END                                               RCTN0111      000727
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@FOR,S LEWIS.RKTOUT,LEWIS.RKTOUT
N.A  E3 -10/25/79-17:39:33 (9,)

   SUBROUTINE RKTOUT     ENTRY POINT 000521

   STORAGE USED: CODE(1) 000530; DATA(0) 000120; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003     CONSTS 000006
    0004     POINTS 000335
    0005     SPECES 012120
    0006     INDX   000041
    0007     PERF   000166
    0010     OUPT   000073
    0011     CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0012     OUT1
    0013     VARFMT
    0014     OUT2
    0015     GAMEFF
    0016     OUT3
    0017     NWDU$
    0020     NIO2$
    0021     NIO1$
    0022     SQRT
    0023     NIO3$
    0024     NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001     000057 144G        0000     000066 150F        0001     000070 152G        0001     000115 166G        0001     000144 176G
    0001     000176 200L        0000     000075 208F        0001     000231 220G        0001     000416 220L        0001     000257 234G
    0001     000312 252G        0001     000334 264G        0001     000344 272G        0001     000362 303G        0001     000505 312L
    0001     000412 317G        0001     000423 324G        0001     000441 335G        0001     000462 346G        0001     000501 356G
    0000     000006 37F         0000     000027 38F         0000     000056 40F         0000     000047 737F        0005     006034 A
    0007 R   000150 AEAT        0007 R   000133 APP         0003 R   000000 ATMN        0000 R   000002 AW          0006     000036 CALCH
    0005     000000 COEF        0006     000001 CONVG       0004     000032 CPR         0000 R   000005 CSTR        0005     005670 DELN
    0011     000002 DEMAND      0004     000064 DLVPT       0004     000047 DLVTP       0005     002734 LN          0005     005360 ENLN
    0007 L   000165 EQL         0010 R   000002 FA          0010     000003 FAP         0010 R   000005 FB          0010 R   000006 FC
    0010     000007 FCF         0010 R   000012 FCST        0010 R   000014 FCV         0010 R   000015 FG          0010 R   000017 FGE
    0010 R   000020 FGV         0010     000021 FH          0010 R   000023 FI          0010 R   000025 FIV         0010     000027 FM
    0010 R   000031 FMI         0010 R   000050 FN          0010 R   000052 FOUR        0010 R   000053 FP          0010     000054 FS
    0010     000056 FSV         0010     000057 FT          0010     000061 FTK         0010     000063 FV          0010 R   000065 FVEL
    0011 R   000001 F13         0010 R   000000 F9X         0004 R   000101 GAMMAS      0003 R   000001 GMET        0011     000000 GRAPH
    0006     000003 HP          0004 R   000000 HSUM        0005 R   005524 HO          0000 I   000004 I           0006     000030 IC
    0006     000000 IDCHOL      0006     000015 IMAT        0000     000103 INJP$       0006     000023 IONS        0006     000021 IP
    0006     000037 ICSAVE      0006     000016 IC1         0006     000005 ISV         0006 I   000034 IT          0005     011444 IUSE
    0006     000026 JLIQ        0011 I   000001 JOUT        0006     000025 JSOL        0006     000031 JS1         0000 I   000003 K
    0006     000014 KMAT        0006     000040 LSAVE       0006     000006 MOLES       0006     000024 NC          0006     000022 NEWR
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0006    000035 NFZ        0006    000012 NLM       0006    000017 NOF        0006    000020 NOMIT      0006    000007 NP
0006  I 000011 NPT        0006    000027 NREAC     0006    000013 NS         0000  I 000000 NSPP1      0006    000010 NT
0010  R 000067 ONE        0004    000116 P         0003  R 000002 PATM       0007    000000 PCP        0004  R 000217 PPP
0003    000003 RBAR       0003  R 000004 RBR       0003    000005 RVR        0005    002570 S          0006    000033 SHOCK
0005    011754 SLN        0004  R 000251 SONVEL    0006    000004 SP         0007  R 000047 SPIM       0004    000015 SSUM
0005    010770 SUB        0007    000101 SUBAR     0007    000116 SUPAR      0004  R 000150 T          0000  R 000001 TEM
0005    011610 TEMP       0010  R 000070 THREE     0004    000320 TOTN       0006    000002 TP         0004  R 000266 TTT
0010  R 000071 TWO        0004  R 000202 V         0007  R 000064 VACI       0004    000303 VLM        0007  R 000032 VMOC
0006    000032 VOL        0004  R 000234 WM        0010    000072 ZERO


00101            SUBROUTINE RKTOUT (IGAM)                                                           000000
00101      C                                                                                        000000
00101      C  ROCKET PERFORMANCE PARAMETERS                                                         000000
00101      C                                                                          ROUTU001      000000
00103            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                          /CONSTS/      000000
00104            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                        000000
00104           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                   000000
00104           2 ,VLM(13),TOTN(13)                                                                 000000
00104      C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                    000000
00104      C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                     000000
00105            INCLUDE SPECPK                                                                     000000
00111            COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,        /INDX/      000000
00111           1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,       /INDX/      000000
00111           2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE         /INDX/      000000
00112            COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),            /PERF/      000000
00112           1              SUPAR(13),APP(13),AEAT(13),EQL                           /PERF/      000000
00113            COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCSI(2),FCV,FG(2),        /OUPT/      000000
00113           1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR,     /OUPT/      000000
00113           2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,       /OUPT/      000000
00113           3              TWO,ZERO                                                 /OUPT/      000000
00113      C                                                                                        000000
00114            COMMON /CCC/ GRAPH,JOUT,DEMAND                                                     000000
00114      C                                                                                        000000
00115            LOGICAL EQL                                                                        000000
00115      C                                                                                        000000
00116            IF(EQL) WRITE(JOUT,37)                                                             000000
00121         37 FORMAT(1H1/24X,84HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRROCK0090         000006
00121           1IUM COMPOSITION DURING EXPANSION         //)                                       000006
00122            IF (.NOT.EQL) WRITE(JOUT,38)                                                       000006
00125         38 FORMAT(1H1,26X,76HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN CROCK0107         000017
00125           1OMPOSITION DURING EXPANSION         //)                              ROCK0108      000017
00126            IF(TTT(1).EQ.T(IT)) WRITE(JOUT,737)                                                000017
00131        737 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE        )                                 000030
00132            TEM = FATM*PPP(1)                                                                  000030
00133            AW = ATMN*PPP(1)                                                                   000033
00134            WRITE(JOUT,40) TEM,AW                                                              000036
00140         40 FORMAT (5H PC =,F10.3,7H PSIA =,1PE13.6,7H N/M**2)                                 000045
00141            CALL OUT1                                                                          000045
00142            K = NPT - 2                                                                        000047
00143            DO 20 I = 1,K                                                                      000052
00146         20 V(I) = 4HEXIT                                                                      000057
00150            WRITE(JOUT,150) (V(I), I = 1,K)                                                    000061
00156        150 FORMAT (1H0,16X,16HCHAMBER    THROAT,11(5X,A4))                          RKT01590      000073
```

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00156    44*     C      PRESSURE RATIOS                                                     OUTPU030    000073
00157    45*            FMT(3) = ONE                                                                    000073
00160    46*            CALL VARFMT (APP,NPT)                                                           000075
00161    47*            WRITE(JOUT,FMT) FP,FB,FB,(APP(I), I = 1,NPT)                                    000101
00172    48*            CALL OUT2                                                                       000120
00173    49*            IF (NPT .LT. 2)  GO TO 312                                                      000122
00175    50*            DO 202 K=2,NPT                                                      ROUTU028    000132
00200    51*            SPIM(K) = SQRT(2.0*RBR*(HSUM(1) - HSUM(K)))/GMET                                000144
00200    52*     C  AW (A/W) IN UNITS OF SEC/ATM                                                        000144
00201    53*            AW = RBR*TTT(K)/(PPP(K)*WM(K)*SPIM(K)*GMET**2)                                  000155
00202    54*            IF(K.NE.2)GO TO 200                                                 ROUTU031    000165
00204    55*            CSTR = GMET*AW*PPP(1)                                                           000170
00205    56*            AEAT(2) = 1.                                                                    000173
00206    57*       200 VACI(K)=SPIM(K)+PPP(K)*AW                                                        000176
00207    58*            IF (SONVEL(K) .GT. 0.0)  VMOC(K) = GMET*SPIM(K)/SONVEL(K)                       000201
00211    59*       202  V(K) = GMET*SPIM(K)                                                             000210
00213    60*            V(1) = 0.0                                                                      000215
00214    61*            WRITE(JOUT,FMT) FGV,FVEL,(V(I), I = 1,NPT)                                      000216
00214    62*     C    MACH NUMBER                                                       ROUTU040    000216
00224    63*            FMT(4) = FOUR                                                                   000234
00225    64*            VMOC(1)=0.                                                          ROUTU042    000236
00226    65*            IF (GAMMAS(2) .LE. 0.0)  VMOC(2) = 0.0                                          000237
00230    66*            WRITE(JOUT,FMT) FN,FB,(VMOC(I), I = 1,NPT)                                      000243
00240    67*            WRITE(JOUT,208)                                                                 000262
00242    68*       208 FORMAT (1H )                                                     ROUTU048    000267
00242    69*     C    AREA RATIO                                                        ROUTU062    000267
00243    70*            CALL VARFMT (AEAT,NPT)                                                          000267
00244    71*            FMT(3) = F9X                                                                    000275
00245    72*            WRITE(JOUT,FMT) FA,FB,FB,(AEAT(I), I = 2,NPT)                                   000277
00245    73*     C      CSTAR                                                                           000277
00256    74*            FMT(4) = F13                                                                    000315
00257    75*            FMT(5) = TWO                                                                    000317
00260    76*            WRITE(JOUT,FMT) FCST,FB,(CSTR, I = 2,NPT)                                       000321
00260    77*     C    CF - THRUST COEFICIENT                                            ROUTU055    000321
00270    78*            FMT(5) = FOUR                                                                   000337
00271    79*            DO 212  I=2,NPT                                                     ROUT0057    000344
00274    80*       212  V(I) = GMET*SPIM(I)/CSTR                                                        000344
00276    81*            WRITE(JOUT,FMT) FC,FB,FB,(V(I), I = 2,NPT)                                      000350
00307    82*            IF (IGAM .EQ. 0)  GO TO 220                                                     000365
00307    83*     C      EFFECTIVE GAMMA                                                                 000365
00311    84*            CALL GAMEFF (V,GAMMAS,APP,NPT,HO)                                               000367
00312    85*            WRITE(JOUT,FMT) FG(1),FGE,FB,(HO(I), I = 2,NPT)                                 000376
00312    86*     C      VACUUM THRUST COEFFICIENT                                           RKT01050    000376
00323    87*       220  DO 230 I = 2,NPT                                                                000416
00326    88*       230  V(I) = GMET*VACI(I)/CSTR                                                        000423
00330    89*            WRITE(JOUT,FMT) FCV,FB,FB,(V(I), I = 2,NPT)                                     000427
00330    90*     C    VACUUM IMPULSE                                                    ROUTU067    000427
00341    91*            FMT(5) = THREE                                                                  000444
00342    92*            WRITE(JOUT,FMT) FIV,FB,(VACI(I), I = 2,NPT)                                     000446
00342    93*     C    SPECIFIC IMPULSE                                                  ROUTU071    000446
00352    94*            WRITE(JOUT,FMT) FI,FB,(SPIM(I), I = 2,NPT)                                      000465
00352    95*     C      FROZEN MOLE FRACTION OUTPUT MOVED TO SUBROUTINE OUT3            RKT01480    000465
00362    96*       312 CALL OUT3                                                                        000505
00363    97*            RETURN                                                                          000506
00364    98*            END                                                                             000527
END FOR
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@FOR,S LEWIS.ROCKET,LEWIS.ROCKET
NSA  E3 -10/25/79-17:39:40 (0,)

    SUBROUTINE ROCKET     ENTRY POINT 001303

    STORAGE USED: CODE(1) 001312; DATA(0) 000222; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003    CONSTS 000006
     0004    POINTS 000335
     0005    MISC   001264
     0006    INDX   000041
     0007    PERF   000166
     0010    CCC    000003

    EXTERNAL REFERENCES (BLOCK, NAME)

     0011    NEWOF
     0012    FROZEN
     0013    EQLBRM
     0014    RKTOUT
     0015    SAVE
     0016    NRNL$
     0017    NWNL$
     0020    XPRR
     0021    NWDU$
     0022    NIO2$
     0023    ALOG
     0024    EXP
     0025    XPDR
     0026    SQRT
     0027    NERR3$

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001     000013 125G      0001     000155 1332L     0001     000030 141G      0001     000047 153G      0000     000076 1811F
     0001     000275 191L      0001     000413 192L      0000     000073 194F      0001     000254 195L      0001     000121 200G
     0001     000021 303L      0001     000040 306L      0001     000076 321L      0001     000115 322L      0001     000146 331L
     0001     000153 332L      0001     000170 333L      0001     000206 334L      0001     000603 799L      0001     000531 800L
     0001     000756 802L      0001     000633 805L      0001     000676 809L      0001     000646 810L      0001     001002 820L
     0000     000117 821F      0001     001010 830L      0001     001036 834L      0001     001046 835L      0001     001050 859L
     0001     001054 860L      0000     000131 862F      0000     000160 865F      0001     001114 870L      0001     001130 880L
     0001     000452 899L      0001     000472 900L      0000     000065 923F      0001     000411 925L      0001     001164 990L
     0001     001225 997L      0001     001257 999L      0007 R 000150 AEAT      0000 R 000037 AEATL     0005     000570 AM
     0005     000624 AM1       0005     000741 ANUM      0007 R 000133 APP       0000 R 000035 APPL      0000 R 000033 ARATIO
     0000 L 000005 AREA      0000 D 000001 ASQ       0003     000000 ATMN      0005     000004 ATOM      0000 R 000030 AWT
     0005     000502 B0        0005     000521 BOP       0006     000036 CALCH     0006     000001 CONVG     0004 R 000032 CPR
     0000 R 000023 CPWF      0005     000625 CPR1      0005 R 000564 CPSUM     0005     000604 DATA      0010     000002 DEMAND
     0005     001167 DENS      0000 R 000026 DH        0000 R 000032 DLNP      0000 R 000040 DLNPE     0000 R 000027 DLT
     0004     000064 DLVPT     0004 R 000047 DLVTP     0000 R 000034 ELN       0005     001263 ENLSAV    0005 R 000000 ENN
     0005     001261 ENNL      0005     001262 ENSAVE    0005     001073 ENTH      0007 L 000165 EQL       0005     000566 EQRAT
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0005     001112 FAZ         0005     001150 FOX         0000 L 000006 FROZ        0004 R 000101 GAMMAS      0003     000001 GMET
0010     000000 GRAPH       0006 L 000003 HP          0005     000572 HPP         0005     000567 HSUBU       0004 R 000000 HSUM
0000 I 000012 I           0006     000030 IC          0000 I 000000 ICASE       0006 I 000000 IDEBUG      0000 I 000011 IGAM
0006     000015 IMAT        0000     000206 INJPS       0000 I 000016 IOF         0006     000023 IONS        0006 I 000021 IP
0000 I 000022 IPP         0006     000037 IQSAVE      0006     000016 IQI         0000 I 000020 ISUB        0000 I 000021 ISUP
0006 I 000005 ISV         0006 I 000034 IT          0000 I 000017 ITNUM       0000 I 000025 ITROT       0006     000026 JLIQ
0010 I 000001 JOUT        0006 I 000025 JSOL        0006     000031 JSI         0006     000014 KMAT        0005     000463 LLMT
0006     000040 LSAVE       0006     000006 MOLES       0005     000626 NAME        0006     000024 NC          0006     000022 NEWR
0006 I 000035 NFZ         0006     000012 NLM         0006 I 000017 NOF         0006     000020 NOMIT       0006 I 000007 NP
0000 I 000013 NPP         0006 I 000011 NPT         0006     000027 NREAC       0006     000013 NS          0000 I 000014 NSUB
0000 I 000015 NSUP        0006 I 000010 NT          0005 R 000565 OF          0005 R 001227 OXF         0004 R 000116 P
0003     000002 PATM        0007 R 000000 PCP         0000 R 000031 PCPLT       0005     001054 PECWT       0005 R 000563 PP
0004 R 000217 PPP         0003     000003 RBAR        0003 R 000004 RBR         0005     000574 RH          0005     001206 RHOP
0000     000041 RKTINP      0005     001207 RMW         0005     001131 RTEMP       0003     000005 RVR         0000 L 000007 SEQL
0006     000033 SHOCK       0004     000251 SONVEL      0006 L 000004 SP          0007     000047 SPIM        0004 R 000015 SSUM
0007 R 000101 SUBAR       0005     000001 SUMN        0007 R 000116 SUPAR       0005 R 000003 SO          0004 R 000150 T
0000 L 000010 THI         0005     000562 THIGH       0005     001226 TLN         0005     000560 TLOW        0005     000557 TM
0000 R 000024 TMELT       0005     000561 TMID        0000 R 000036 TOL         0004     000320 TOTN        0006 L 000002 TP
0005 R 000002 TT          0004 R 000266 TTT         0000 D 000003 USQ         0004     000202 V           0007     000064 VACI
0004     000303 VLM         0005     000576 VMIN        0007     000032 VMOC        0006     000032 VOL         0005     000600 VPLS
0004 R 000234 WM          0005     000602 WP
```

```
00101      1*           SUBROUTINE ROCKET                                                  ROCK0002    000000
00101      2*     C                                                                        ROCK0001    000000
00101      3*     C     ROCKET PERFORMANCE                                                 ROCK0004    000000
00101      4*     C                                                                                    000000
00103      5*           COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                        /CONSTS/    000000
00104      6*           COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                    000000
00104      7*          1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)               000000
00104      8*          2 ,VLM(13),TOTN(13)                                                             000000
00105      9*           COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),           /MISC/     000000
00105     10*          1              BOF(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,       /MISC/     000000
00105     11*          2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),       /MISC/     000000
00105     12*          3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),    /MISC/     000000
00105     13*          4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,     /MISC/     000000
00105     14*          5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                /MISC/     000000
00106     15*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/     000000
00106     16*          1              KMAT,IMAT,IQI,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,    /INDX/     000000
00106     17*          2              NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE      /INDX/     000000
00107     18*           COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACT(13),SUBAR(13),        /PERF/     000000
00107     19*          1              SUPAR(13),APP(13),AEAT(13),EQL                        /PERF/     000000
00107     20*     C                                                                                    000000
00110     21*              COMMON /CCC/ GRAPH,JOUT,DEMAND                                              000000
00110     22*     C                                                                                    000000
00111     23*           DATA ICASE/0/                                                                  000000
00113     24*           DOUBLE PRECISION ASQ,USQ                                                       000000
00114     25*           LOGICAL AREA,EQL,FROZ,HP,SEQL,SP,THI,TP                                        000000
00114     26*     C                                                                                    000000
00115     27*           NAMELIST /RKTINP/ EQL,FROZ,IGAM,PCP,SUBAR,SUPAR                    /RKTINP/    000000
00115     28*     C                                                                                    000000
00115     29*           NFZ = 1                                                                        000000
00117     30*           APP(1) = 1.                                                                    000001
00103     31*           IF (ICASE .GT. 0)  GO TO 303                                                   000003
```

```
00122              ICASE = 1                                                           000006
00123              IGAM = 0                                                            000007
00124              DO 300 I=1,26                                                       000013
00127              PCP(I)= 0.                                                          000013
00130        300   SUBAR(I) = 0.0                                                      000013
00132              EQL = .TRUE.                                                        000015
00133              FROZ = .FALSE.                                                      000017
00134        303   READ (5,RKTINP)                                                     000021
00137              NPP = 0                                                             000024
00140              DO 305 I = 1,26                                                     000030
00143              IF (PCP(I) .LE. 0.0)  GO TO 306                                     000030
00145        305   NPP = I                                                             000033
00147         306  NPP = NPP+2                                                         000040
00150              NSUB = 0                                                            000042
00151              NSUP = 0                                                            000043
00152              DO 320  I=1,13                                                      000047
00155              IF (SUBAR(I) .GT. 0.0)  NSUB = NSUB + 1                             000047
00157        320   IF (SUPAR(I) .GT. 0.0)  NSUP = NSUP + 1                             000054
00162              WRITE(JOUT,RKTINP)                                                  000064
00165              SEQL = EQL                                                          000070
00166              IOF = 0                                                             000072
00167              TT = 3800.                                                          000073
00167       C      LOOP FOR EACH O/F                                                   000073
00170         321  IT = 1                                                              000076
00171              IOF = IOF + 1                                                       000077
00172              OF = OXF(IOF)                                                       000102
00173              CALL NEWOF                                                          000104
00174              IF (T(1) .LE. 0.0)  GO TO 322                                       000106
00176              TT = T(IT)                                                          000112
00176       C      LOOP FOR CHAMBER PRESSURES                                          000112
00177         322  DO 998 IP = 1,NP                                                    000115
00202              ITNUM = 0                                                           000121
00203              AREA = .FALSE.                                                      000122
00204              IF (T(1) .LE. 0.0)  HP = .TRUE.                                     000123
00206              IF (T(1) .GT. 0.0)  TP = .TRUE.                                     000130
00210              SP = .FALSE.                                                        000135
00211              EQL = .TRUE.                                                        000136
00212              ISUB = 1                                                            000140
00213              ISUP = 1                                                            000141
00214              PP = P(IP)                                                          000142
00215              IPP = 1                                                             000144
00215       C      LOOP FOR PRESSURE RATIOS                                            000144
00216         331  IF(EQL)  GO TO 332                                                  000146
00220              CALL FROZEN                                                         000147
00221              GO TO 1332                                                          000151
00222         332  CALL EQLBRM                                                         000153
00222       C      IT = 0 IF NO CONVERGENCE                                            000153
00223       1332   IF (IT .GT. 0.0)  GO TO 333                                         000155
00225              IF (NPT .LT. 2)  RETURN                                             000157
00227              GO TO 900                                                           000166
00230         333  IF(IPP.GT.1) GO TO 195                                              000170
00230       C      COMBUSTION CHAMBER                                      ROCKU060    000170
00232              EQL = SEQL                                                          000173
00233              TP = .FALSE.                                            ROCKU062    000175
00234              HP = .FALSE.                                            ROCKU063    000176
00235              SP = .TRUE.                                             ROCKU064    000177
```

```
00236            SD = SSUM(1)                                                                   000201
00237            CPRF = CFSUM                                                                   000203
00240       334  TMELT=0.                                                                       000206
00241            ITROT = 3                                                                      000206
00242            THI = .FALSE.                                                                  000210
00243            APP(2)=((GAMMAS(1)+1.)/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))        ROCK0066         000211
00244            IF(EQL)  WRITE(JOUT,194) APP(2)                                                000227
00250            PP = PPP(1)/APP(2)                                                             000237
00251            TT = 2.*TT/(GAMMAS(1)+1.)                                                      000242
00252            ISV = 1                                                                        000250
00253            GO TO 870                                                                      000252
00254       195  USQ = 2.0*RBR*(HSUM(1) - HSUM(NPT))                                            000254
00255            IF (IPP.GT.2) GO TO 900                                                        000264
00255     C      THROAT                                                        ROCK0073         000264
00257            IF (.NOT. THI)  GO TO 191                                                      000270
00261            GAMMAS(2) = 0.                                                                 000272
00262            GO TO 899                                                                      000273
00263       191  ASQ = RBR*GAMMAS(2)*TT*ENN                                                     000275
00264            IF(IDEBUG.EQ.1.OR.IDEBUG.EQ.2)  WRITE(JOUT,923)USQ,ASQ                         000304
00271       923  FORMAT(5H0USQ=,E15.8,5X,4HASQ=,E15.8)                                          000327
00272            DH = (USQ-ASQ)/ASQ                                                             000327
00273            IF(DH.LT.0.)  DH=-DH                                                           000334
00275            IF(DH.LE.0.4E-4.OR.ITROT.EQ.0)  GO TO 699                                      000341
00277            IF (JSOL .NE. 0)  GO TO 925                                                    000354
00301            IF (TMELT .LE. 0.0)  GO TO 192                                                 000356
00303            DLT = ALOG(TMELT/TT)                                                           000361
00304            PP = PP*EXP(DLT*CPR(2)/(ENN*DLVTP(2)))                                         000370
00305            APP(2) = P(IP)/PP                                                              000402
00306            THI = .TRUE.                                                                   000405
00307            GO TO 331                                                                      000407
00310       925  TMELT = TT                                                                     000411
00311       192  APP(2) = APP(2)/(1.0 + (USQ - ASQ)/(ENN*(GAMMAS(2) + 1.0)*RBR*TT))             000413
00312            PP = P(IP)/APP(2)                                                              000432
00313            ITROT = ITROT-1                                               ROCK0079         000435
00314            IF(EQL)  WRITE(JOUT,194) APP(2)                                                000440
00320       194  FORMAT(7H PC/PT=,F9.6)                                                         000450
00321            GO TO 331                                                                      000450
00322       899  AWT =ENN*TT/(PP*USQ**.5)                                                       000452
00323            PCPLT = ALOG(APP(2))                                                           000465
00324       900  ISV =0                                                                         000472
00325            IF (TT .LE. 0.0)  GO TO 860                                                    000473
00327            AEAT(NPT) = ENN*TT/(PP*USQ**.5*AWT)                                            000476
00330            IF(AREA)  GO TO 800                                                            000514
00332            IF(IPP.LT.NPP)  GO TO 859                                                      000516
00334            IF((NSUB+NSUP).EQ.0)  GO TO 860                                                000522
00336            AREA = .TRUE.                                                                  000526
00336     C      PCP ESTIMATES FOR AREA RATIOS                                                  000526
00337       800  IF(ITNUM.NE.0)  GO TO 810                                                      000531
00341            DLNP = 1.                                                                      000534
00342            ITNUM = 1                                                                      000536
00343            ARATIO = SUBAR(ISUB)                                                           000540
00344            IF(NSUB.LE.0)  ARATIO=SUPAR(ISUP)                                              000544
00346            ELN = ALOG(ARATIO)                                                             000552
00347            IF(NSUB.LE.0)  GO TO 799                                                       000556
00351            APPL = PCPLT/(SUBAR(ISUB)+(10.587*ELN**2+9.454)*ELN)                           000561
00352            IF(ARATIO.LT.1.09)  APPL=.9*APPL                                               000572
```

```
00354          GO TO 859                                                                   000601
00355      799 IF(SUPAR(ISUP).LT.2.)  GO TO 805                                            000603
00357          IF(ISUP.GT.1.AND.SUPAR(ISUP-1).GE.2.)  GO TO 802                            000607
00361          APPL = GAMMAS(2)*ELN*1.4                                                    000625
00362          GO TO 859                                                                   000631
00363      805 APPL = SQRT(ELN*(1.535+3.294*ELN))*PCPLT                                    000633
00364          GO TO 859                                                                   000644
00365      810 IF (IDEBUG .LE. 0 .OR. NPT .LT. IDEBUG)  GO TO 809                          000646
00367          WRITE(JOUT,1811)ITNUM,ARATIO,AEAT(NPT),APP(NPT),DLNP                        000662
00376     1811 FORMAT (6H0ITER=,I2,5X,15HASSIGNED AE/AT=,F15.8,5X,6HAE/AT=,F15.8,           000676
00376         15X,5HPC/P=,F15.8,5X,11HDELTA LN P=,F15.8)                                  000676
00377      809 TOL = 1.0E-5                                                                000676
00400          IF (ARATIO .GE. 10.0)  TOL = 4.0E-5                                         000701
00402          IF (ABS(AEAT(NPT) - ARATIO)/ARATIO .LE. TOL)  GO TO 830                     000707
00404          IF (ABS(DLNP) .LT. 4.0E-6)  GO TO 830                                       000717
00406          AEATL= ALOG(AEAT(NPT))                                                      000723
00407          ITNUM = ITNUM + 1                                                           000731
00410          IF (ITNUM .GT. 25)  GO TO 820                                               000734
00412          ASQ = RBR*GAMMAS(NPT)*ENN*TT                                                000737
00413          DLNPE = GAMMAS(NPT)*USQ/(USQ-ASQ)                                           000747
00414      802 DLNP = DLNPE*ELN-DLNPE*AEATL                                                000756
00415          APPL = APPL + DLNP                                                          000764
00416          IF(ITNUM.EQ.1)  GO TO 859                                                   000766
00420          APP(NPT) = EXP(APPL)                                                        000771
00421          PP = P(IP)/APP(NPT)                                                         000775
00422          GO TO 331                                                                   001000
00423      820 WRITE(JOUT,821) ARATIO                                                      001002
00426      821 FORMAT (/10X,40HROCKET DID NOT CONVERGE FOR AREA RATIO =,F11.6/)            001010
00427      830 ITNUM = 0                                                                   001010
00430          AEAT(NPT) = ARATIO                                                          001011
00431          IF(NSUB.LE.0)  GO TO 834                                                    001013
00432          ISUB = ISUB+1                                                               001016
00434          IF (ISUB .LE. NSUB)  GO TO 800                                              001021
00436          ISUB = 1                                                                    001024
00437          NSUB = -NSUB                                                                001026
00440          IF(ISUP.LE.NSUP)  GO TO 800                                                 001030
00442          GO TO 835                                                                   001034
00443      834 ISUP = ISUP+1                                                               001036
00444          IF(ISUP.LE.NSUP)  GO TO 800                                                 001040
00446          ISUP = 1                                                                    001043
00447      835 AREA = .FALSE.                                                              001046
00450          GO TO 860                                                                   001046
00451      859 ISV = NPT                                                                   001050
00452          IF(NPT.NE.13)  GO TO 870                                   ROCK0088         001051
00454      860 CALL RKTOUT (IGAM)                                                          001054
00455          IF (TT .LE. 0.0)  ISV = 0                                                   001056
00457          IF (.NOT. EQL .AND. TT .LE. 0.0)  WRITE(JOUT,862)                           001062
00462      862 FORMAT (///2X,125HCALCULATIONS WERE STOPPED IN ROCKET BECAUSE NEXT          001077
00462         1POINT IS MORE THAN 50 DEGREES BELOW TEMPERATURE RANGE OF A CONDENS          001077
00462         .ED SPECIES)                                                                 001077
00463          IF (ISV.EQ.0) GO TO 990                                                     001077
00465          IDEBUG = IDEBUG-13                                                          001101
00466          WRITE(JOUT,865)                                                             001104
00470      865 FORMAT(1H1)                                                                 001111
00471          NPT = 2                                                                     001111
00472      870 NPT = NPT + 1                                              ROCK0121         001114
```

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```
00473           IF(.NOT.EQL)  GO TO 880                                        001116
00475           IF(ISV.EQ.1)  ISV = -1                                         001120
00477           CALL SAVE                                                      001125
00500       880 IPP = IPP+1                                                    001130
00501           IF(NPT.EQ.2)  GO TO 331                                        001133
00503           IF(.NOT.AREA)  APP(NPT)=PCP(IPP-2)                             001136
00505           IF(AREA)  APP(NPT)=EXP(APPL)                                   001147
00507           PP = P(IP)/APP(NPT)                                            001156
00510           GO TO 331                                                      001162
00511       990 IF(IDEBUG.LT.0)  IDEBUG=IDEBUG+13                              001164
00513           IF(NSUB.LT.0)  NSUB=-NSUB                                      001171
00515           IF (.NOT.FROZ.OR..NOT.EQL)  GO TO 997                          001176
00517           CPR(1) = CPRF                                                  001201
00520           GAMMAS(1) = CPRF/(CPRF-1./WM(1))                               001203
00521           TT = TTT(1)                                                    001210
00522           IPP = 1                                                        001212
00523           NPT = 1                                                        001214
00524           CALL SAVE                                                      001215
00525           EQL = .FALSE.                                                  001217
00526           ENN = 1./WM(1)                                                 001220
00527           GO TO 334                                                      001223
00530       997 NPT = 1                                                        001225
00531           WRITE(JOUT,865)                                                001226
00533           IF (SEQL)  CALL SAVE                                           001233
00535      998  TT = TTT(1)                                                    001237
00537           IF(IT.GE.NT)  GO TO 999                                        001243
00541           IT = IT+1                                                      001247
00542           TT = T(IT)                                                     001253
00543           GO TO 322                                                      001255
00544      999  IF (IOF .GE. NOF)  RETURN                                      001257
00546           GO TO 321                                                      001265
00547           END                                                ROCKU129    001311
END FOR
```

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```
@FOR,S LEWIS.RREAD,LEWIS.RREAD
FTN  E -10/25/79-17:37:49 (17,)

 SUBROUTINE RREAD      ENTRY POINT 001255

 STORAGE USED: CODE(1) 001273; DATA(0) 001031; BLANK COMMON(2) 000000

 EXTERNAL REFERENCES (BLOCK, NAME)

  0003    ROYES
  0004    PAGIT
  0005    CHRS12
  0006    GOUT
  0007    NNCOD$
  0010    RDATA1
  0011    RDATAF
  0012    DMWRTF
  0013    RDCHAR
  0014    NREW$
  0015    NRDU$
  0016    NIO2$
  0017    NIO1$
  0020    NERR2$
  0021    NWDU$
  0022    NWEF$
  0023    NERR3$

 STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

  0001     000010 10L       0001     000260 100L      0001     000343 106L      0001     000405 110L      0001     000470 120L
  0001     000522 130L      0001     000556 140L      0001     000574 150L      0001     000615 160L      0001     000633 170L
  0001     000032 172G      0001     000037 176G      0001     000654 200L      0001     000107 225G      0001     000116 232G
  0001     000720 300L      0001     000275 306G      0001     001003 310L      0001     000334 327G      0001     001033 330L
  0001     001061 340L      0001     000424 350G      0001     001100 350L      0001     001115 360L      0001     000452 361G
  0001     001134 370L      0001     001152 400L      0001     000667 433G      0001     000670 436G      0001     000741 464G
  0001     000766 475G      0001     000060 50L       0001     001170 551G      0001     001175 555G      0001     000160 70L
  0000     000722 800F      0000     000723 801F      0000     000736 802F      0000     000752 803F      0001     000221 90L
  0001     000255 95L       0000 R 000113 ANUM      0000 R 000360 DENS      0000 R 000264 ENTH      0000 R 000571 EXMP1A
  0000 R 000604 EXMP1B    0000 R 000614 EXMP2     0000 R 000622 EXMP2B    0000 R 000627 EXMP3     0000 R 000634 EXMP3B
  0000 R 000643 EXMP4     0000 R 000647 EXMP5     0000 R 000653 EXMP6     0000 R 000660 EXMP7     0000 R 000303 FAZ
  0000 R 000341 FOX       0000 I 000715 I         0000 I 000721 ICHNG     0000 I 000712 IDUM      0000     001006 INJP$
  0000 I 000713 IO        0000 I 000717 IOPT      0000 I 000467 IOUT      0000 I 000664 IREACT    0000 I 000716 J
  0000 I 000702 LINE0     0000 I 000377 LINE1     0000 I 000424 LINE2     0000 I 000447 LINE3     0000 I 000514 MODIFY
  0000 I 000531 MOUMEN    0000 I 000245 MOLE      0000 I 000720 N         0000 I 000000 NAME      0000 I 000714 NREAC
  0000 R 000226 RECWT     0000 R 000670 RDUM      0003 L 000000 ROYES     0000 R 000322 RTEMP


 00101      1*          SUBROUTINE RREAD(FIRST)                                              000000
 00102      2*          LOGICAL FIRST,ROYES                                                  000000
 00103      3*    C                                                                          000000
```

```
00103     C        USE MIFS INPUT ROUTINES TO READ REACTANT CARDS (STORE ON FILE 8)           000000
00103     C                                                                                   000000
00103     C        DATA ARRAYS FOR REACTANT CARDS                                             000000
00104              DIMENSION NAME(15,5),ANUM(15,5),PECWT(15),MOLE(15),ENTH(15),               000000
00104            1 FAZ(15),RTEMP(15),FOX(15),DENS(15)                                         000000
00104     C                                                                                   000000
00104     C        ARRAYS FOR DATA MENU'S                                                     000000
00105              DIMENSION LINE1(21),LINE2(19),LINE3(16),IOUT(21),MODIFY(13)                000000
00106              DIMENSION MODMEN(4,8),EXMP1A(11),EXMP1B(8),EXMP2(6),EXMP2B(5),             000000
00106            1 EXMP3(5),EXMP3B(7),EXMP4(4),EXMP5(4),EXMP6(5),EXMP7(4),                    000000
00106            . IREACT(4),RDUM(10),LINE0(8)                                                000000
00106     C                                                                                   000000
00106     C        SET DATA ARRAYS FOR MENUS                                                  000000
00107              DATA LINE0/6HTYPE  ,6HYES  1,6H0 READ,6H IN PR,6HEVIOUS,                   000000
00107            1 6H REACT,6HANT SE,6HT       /                                              000000
00111              DATA LINE1/6H INDEX,4*6H       ,6HREACTA,6HNT(*) ,3*6H       ,             000000
00111            1 6H     R,6HEL WT/,6H   MOL,6HE  ENT,6HHALPY/,6H   PHA,6HSE  TE,            000000
00111            2 6HMP,K  ,6H FUEL/,6H  DENS,6HITY    /                                      000000
00113              DATA LINE2/10*6H       ,6H      N,6H0 MOLE,6HS      ,6H   INT,             000000
00113            1 6H ENERG,6HY      ,2*6H       ,6H OXID /                                   000000
00115              DATA LINE3/8*6H       ,6H  *  0,6H0  IND,6HICATES,6H ENTHA,                000000
00115            1 6HLPY TO,6H BE CA,6HLCULAT,6HED       /                                    000000
00117              DATA MODMEN/24H 1-REACTANT FORMULA      ,                                  000000
00117            1 24H 2-REL WT/NO MOLES        ,24H 3-ENTHALPY/ENERGY//CALC ,                000000
00117            2 24H 4-PHASE (S-L-G)          ,24H 5-TEMPERATURE (K)       ,                000000
00117            3 24H 6-FUEL,OXIDIZER (F/O)  ,24H 7-DENSITY (G/CM3)        ,                 000000
00117            4 24H RETURN TO CONTINUE      /                                              000000
00121              DATA EXMP1A/36H TYPE CHEMICAL FORMULA THIS REACTANT,                       000000
00121            1 30H, HOLLERINTH CODE FOR SYMBOLS /                                         000000
00123             DATA EXMP1B/48H EXAMPLE CARBON TETRACHLORIDE  1HC 1. 2HCL 4.   /            000000
00125              DATA EXMP2/36H TYPE REL WEIGHT/NUMBER OF MOLES     /                       000000
00127              DATA EXMP2B/30H TYPE YES IF VALUE IS MOLES   /                             000000
00131              DATA EXMP3/30H TYPE ENTHALPY/INTERNAL ENERGY/                              000000
00133              DATA EXMP3B/42H TYPE YES IF ENTHALPY TO BE CALCULATED     /                000000
00135              DATA EXMP4/24H TYPE PHASE (S-L-G)     /                                    000000
00137              DATA EXMP5/24H TYPE TEMPERATURE (K)   /                                    000000
00141              DATA EXMP6/30H TYPE FUEL/OXIDIZER (F/O)      /                             000000
00142              DATA EXMP7/24H TYPE DENSITY (G/CC)    /                                    000000
00145              DATA MODIFY/6H TYPE ,6H 1, 2,,6HOR 3  ,6HTO MOD,6HIFY, D,                  000000
00145            1 6HELETE,,6H OR AD,6HD A RE,6HACTANT,6H (RETU,6HRN TO ,                     000000
00145            2 6HCONTIN,6HUE)   /                                                         000000
00147              DATA IREACT/24H TYPE REACTANT NUMBER   /                                   000000
00151              DATA IDUM/1H /                                                             000000
00153              DATA IO/8/                                                                 000000
00153     C                                                                                   000000
00155              NREAC=0                                                                    000000
00155     C                                                                                   000000
00155     C        FOR FIRST PASS DO NOT CHECK SAVED DATA                                     000000
00156              IF(.NOT.FIRST) GO TO 10                                                    000000
00160              IF(.NOT.RDYES(LINE0,43)) GO TO 50                                          000002
00160     C                                                                                   000002
00160     C        READ IN PRESENT CASE                                                       000002
00162       10     CONTINUE                                                                   000010
00163              REWIND IO                                                                  000010
00164              READ(IO,400) NREAC                                                         000012
00167              IF(NREAC.LT.1) GO TO 50                                                    000020
```

```
00171          DO 25 I=1,NREAC                                                          000024
00174          READ(10,801) (NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),               000032
00174        1 ENTH(I),FAZ(I),RTEMP(I),FOX(I),DENS(I)                                   000032
00212    25    CONTINUE                                                                 000060
00212    C                                                                              000060
00212    C     DISPLAY PRESENT SET OF REACTANTS (ADD IF NONE EXIST)                     000060
00214    50    CONTINUE                                                                 000060
00215          FIRST=.FALSE.                                                            000060
00216          CALL PAGIT                                                               000060
00217          CALL CHRSIZ(4)                                                           000062
00220          IF(NREAC.LT.1) GO TO 300                                                 000065
00222          CALL GOUT(LINE1,125)                                                     000071
00223          CALL GOUT(LINE2,114)                                                     000075
00224          DO 60 I=1,NREAC                                                          000107
00227          ENCODE(802,IOUT)I,(NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),          000107
00227        1 ENTH(I),FAZ(I),RTEMP(I),FOX(I),DENS(I)                                   000107
00244          CALL GOUT(IOUT,125)                                                      000132
00247    60    CONTINUE                                                                 000143
00250          CALL GOUT(IDUM,1)                                                        000143
00252          CALL GOUT(LINE3,92)                                                      000147
00253          CALL GOUT(IDUM,1)                                                        000153
00254    70    CONTINUE                                                                 000160
00255          CALL GOUT(MODIFY,75)                                                     000160
00256          IOPT=0                                                                   000163
00257          CALL RDATAI(1,IOPT,$70)                                                  000164
00260          IF(IOPT.LT.0 .OR. IOPT.GT.3) GO TO 70                                    000171
00262          IF(IOPT.EQ.0) GO TO 400                                                  000206
00264          GO TO(90,90,300),IOPT                                                    000210
00264    C                                                                              000210
00264    C     SELECT REACTANT NUMBER                                                   000210
00265    90    CONTINUE                                                                 000221
00266          N=1                                                                      000221
00267          IF(NREAC.EQ.1) GO TO 95                                                  000222
00271          N=0                                                                      000224
00272          CALL GOUT(IREACT,24)                                                     000225
00273          CALL RDATAI(1,N,$90)                                                     000231
00274          IF(N.LT.1 .OR. N.GT.NREAC) GO TO 90                                      000236
00276    95    CONTINUE                                                                 000255
00277          IF(IOPT.EQ.2) GO TO 200                                                  000255
00277    C                                                                              000255
00277    C     SELECT MODIFICATION OPTIONS                                              000255
00301    100   CONTINUE                                                                 000260
00302          CALL PAGIT                                                               000260
00303          ENCODE(802,IOUT)N,(NAME(N,J),ANUM(N,J),J=1,5),PECWT(N),MOLE(N),          003261
00303        1 ENTH(N),FAZ(N),RTEMP(N),FOX(N),DENS(N)                                   000261
00322          CALL GOUT(LINE1,125)                                                     000311
00323          CALL GOUT(LINE2,114)                                                     000315
00324          CALL GOUT(IOUT,125)                                                      000321
00325          CALL GOUT(IDUM,1)                                                        003325
00326          DO 105 I=1,8                                                             000334
00331          CALL GOUT(MODMEN(1,I),24)                                                003334
00332    105   CONTINUE                                                                 000343
00334    106   CONTINUE                                                                 000343
00335          ICHNG=0                                                                  000343
00336          CALL RDATAI(1,ICHNG,$106)                                                000343
00337          IF(ICHNG .EQ. 0) GO TO 50                                                000350
```

```
00341             IF(ICHNG.LT.1 .OR. ICHNG.GT.7) GO TO 106                000352
00343             GO TO (110,120,130,140,150,160,170),ICHNG                000370
00344      110    CONTINUE                                                 000405
00345             CALL GOUT(EXMP1A,66)                                     000406
00346             CALL GOUT(EXMP1B,48)                                     000413
00347             DO 112 I=1,5                                             000424
00352             J=(I-1)*2 + 1                                            000424
00353             FLD(0,36,RDUM(J))=FLD(0,36,NAME(N,I))                   000431
00354             RDUM(J+1)=ANUM(N,I)                                      000434
00355      112    CONTINUE                                                 000440
00357             CALL RDATAF(10,ROUM,$110)                                000440
00360             DO 114 I=1,5                                             000452
00363             J=(I-1)*2 + 1                                            000452
00364             FLD(0,36,NAME(N,I))=FLD(0,36,RDUM(J))                   000460
00364      C    CALL CHECK(NAME(N,I))                                      000460
00365             ANUM(N,I)=RDUM(J+1)                                      000462
00366      114    CONTINUE                                                 000466
00370             GO TO 100                                                000466
00370      C                                                               000466
00371      120    CONTINUE                                                 000470
00372             CALL DMWRTF(EXMP2,36,PECWT(N),6)                         000470
00373             CALL RDATAF(1,PECWT(N),$120)                             000500
00374             MOLE(N)=1H                                               000507
00375             IF(.NOT.RDYES(EXMP2B,30)) GO TO 100                      000511
00377             MOLE(N)=1HM                                              000515
00400             GO TO 100                                                000520
00400      C                                                               000520
00401      130    CONTINUE                                                 000522
00402             CALL DMWRTF(EXMP3,30,ENTH(N),5)                          000522
00403             CALL RDATAF(1,ENTH(N),$130)                              000532
00404             NAME(N,5)=2H                                             000541
00405             IF(RDYES(EXMP3B,42)) NAME(N,5)=2HOO                      000544
00407             GO TO 100                                                000554
00407      C                                                               000554
00410      140    CONTINUE                                                 000556
00411             CALL GOUT(EXMP4,24)                                      000556
00412             CALL RDCHAR(FAZ(N),1,1,$140)                             000562
00413             GO TO 100                                                000572
00413      C                                                               000572
00414      150    CONTINUE                                                 000574
00415             CALL DMWRTF(EXMP5,24,RTEMP(N),$150)                      000574
00416             CALL RDATAF(1,RTEMP(N),$150)                             000604
00417             GO TO 100                                                000613
00417      C                                                               000613
00420      160    CONTINUE                                                 000615
00421             CALL GOUT(EXMP6,30)                                      000615
00422             CALL RDCHAR(FOX(N),1,1,$160)                             000621
00423             GO TO 100                                                000631
00423      C                                                               000631
00424      170    CONTINUE                                                 000633
00425             CALL DMWRTF(EXMP7,24,DENS(N),5)                          000633
00426             CALL RDATAF(1,DENS(N),$170)                              000643
00427             GO TO 100                                                000657
00427      C                                                               000657
00427      C      DELETE A REACTANT                                        000657
00430      200    CONTINUE                                                 000659
```

```
00431    172*           NREAC=NREAC-1                                           000654
00432    173*           DO 220 I=N,NREAC                                        000660
00435    174*           DO 210 J=1,5                                            000670
00440    175*                NAME(I,J)=NAME(I+1,J)                              000670
00441    176*                ANUM(I,J)=ANUM(I+1,J)                              000671
00442    177*     210   CONTINUE                                                000674
00444    178*           PECWT(I)=PECWT(I+1)                                     000674
00445    179*           MOLE(I)=MOLE(I+1)                                       000676
00446    180*           ENTH(I)=ENTH(I+1)                                       000700
00447    181*           FAZ(I)=FAZ(I+1)                                         000702
00450    182*           RTEMP(I)=RTEMP(I+1)                                     000704
00451    183*           FOX(I)=FOX(I+1)                                         000706
00452    184*           DENS(I)=DENS(I+1)                                       000710
00453    185*     220   CONTINUE                                                000716
00455    186*           GO TO 50                                                000716
00455    187*     C                                                             000716
00455    188*     C     ADD A REACTANT                                          000716
00456    189*     300   CONTINUE                                                000720
00457    190*           NREAC=NREAC+1                                           000720
00460    191*           N=NREAC                                                 000722
00461    192*           CALL GOUT(EXMP1A,66)                                    000723
00462    193*           CALL GOUT(EXMP1B,48)                                    000727
00463    194*           DO 305 I=1,5                                            000741
00466    195*           J=(I-1)*2 + 1                                           000741
00467    196*           RDUM(J)=2H                                              000746
00470    197*           RDUM(J+1)=0.                                            000751
00471    198*     305   CONTINUE                                                000754
00473    199*           CALL RDATAF(10,RDUM,$300)                               000754
00474    200*           DO 307 I=1,5                                            000766
00477    201*           J=(I-1)*2 + 1                                           000766
00500    202*           FLD(0,36,NAME(N,I))=FLD(0,36,RDUM(J))                   000774
00500    203*     C    CALL CHECK(NAME(N,I))                                    000774
00501    204*           ANUM(N,I)=RDUM(J+1)                                     000776
00502    205*     307   CONTINUE                                                001003
00504    206*     310   CONTINUE                                                001003
00505    207*           CALL GOUT(EXMP2,36)                                     001003
00506    208*           PECWT(N)=0.                                             001007
00507    209*           CALL RDATAF(1,PECWT(N),$310)                            001010
00510    210*     320   CONTINUE                                                001017
00511    211*           MOLE(N)=1H                                              001017
00512    212*           IF(RDYES(EXMP2B,30)) MOLE(N)=1HM                        001022
00514    213*     330   CONTINUE                                                001033
00515    214*           CALL GOUT(EXMP3,30)                                     001033
00516    215*           ENTH(N)=0.                                              001037
00517    216*           CALL RDATAF(1,ENTH(N),$330)                             001040
00520    217*           IF(RDYES(EXMP3B,42)) NAME(N,5)=2HOO                     001050
00522    218*     340   CONTINUE                                                001061
00523    219*           CALL GOUT(EXMP4,24)                                     001061
00524    220*           FAZ(N)=1HS                                              001065
00525    221*           CALL RDCHAR(FAZ(N),1,-1,$340)                           001067
00526    222*     350   CONTINUE                                                001100
00527    223*           CALL GOUT(EXMP5,24)                                     001100
00530    224*           RTEMP(N)=0.                                             001104
00531    225*           CALL RDATAF(1,RTEMP(N),$350)                            001105
00532    226*     360   CONTINUE                                                001115
00533    227*           CALL GOUT(EXMP6,30)                                     001115
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00534    228*                 FOX(N)=1HF                                                           001121
00535    229*                 CALL RDCHAR(FOX(N),1,-1,$360)                                        001123
00536    230*      370        CONTINUE                                                             001134
00537    231*                 CALL GOUT(EXMP7,24)                                                  001134
00540    232*                 DENS(N)=0.                                                           001140
00541    233*                 CALL RDATAF(1,DENS(N),$370)                                          001141
00542    234*                 GO TO 50                                                             001150
00542    235*      C                                                                               001150
00542    236*      C        STORE CASE TO FILE 8                                                   001150
00543    237*      400        CONTINUE                                                             001152
00544    238*                 REWIND IO                                                            001152
00545    239*                 WRITE(IO,800) NREAC                                                  001154
00550    240*                 DO 410 I=1,NREAC                                                     001170
00553    241*                 WRITE(IO,801) (NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),          001170
00553    242*            1    ENTH(I),FAZ(I),RTEMP(I),FOX(I),DENS(I)                               001170
00571    243*      410        CONTINUE                                                             001215
00573    244*                 WRITE(IO,803) IDUM                                                   001215
00576    245*                 WRITE(IO,803) IDUM                                                   001223
00601    246*                 ENDFILE IO                                                           001231
00602    247*                 RETURN                                                               001234
00603    248*      800        FORMAT(I3)                                                           001272
00604    249*      801        FORMAT(2X,5(A2,F8.4,2X),/,F10.6,2X,A1,F13.4,4X,A1,F12.3,             001272
00604    250*            1    3X,A1,F12.5,1X)                                                      001272
00605    251*      802        FORMAT(1X,I2,2X,5(A2,F8.4,2X),F10.6,2X,A1,F13.4,4X,A1,F12.3,         001272
00605    252*            1    3X,A1,F12.5,1X)                                                      001272
00606    253*      803        FORMAT(A1)                                                           001272
00607    254*                 END                                                                  001272
END FOR
```

```
@FOR,S LEWIS.SAVE,LEWIS.SAVE
  A  1. -10/25/79-17:40:00 (4,)

    SUBROUTINE SAVE       ENTRY POINT 000463
               NE.OF      ENTRY POINT 000466

    STORAGE USED: CODE(1) 000471; DATA(0) 000065; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003    CONSTS 000006
     0004    HOLLON 000010
     0005    SPECES 012120
     0006    MISC   001264
     0007    INDX   000041
     0010    CCC    000003

    EXTERNAL REFERENCES (BLOCK, NAME)

     0011    HCALC
     0012    EXP
     0013    NWDU$
     0014    NI02$
     0015    NI01$
     0016    NERR3$

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001     000137 100L      0001     000056 13L       0001     000042 131G      0001     000073 15L       0001     000112 20L
     0001     000161 200G      0001     000172 200L      0001     000207 207G      0001     000310 236G      0001     000417 303G
     0001     000127 50L       0000     000013 730F      0001     000273 744L      0001     000304 745L      0001     000340 750L
     0001     000347 760L      0000     000016 770F      0000     000026 780F      0000     000031 785F      0005     006034 A
     0006     000570 AM        0006     000624 AM1       0006     000741 ANUM      0003     000000 ATMN      0006     000004 ATOM
     0006 R   000502 BO        0006 R   000521 BOP       0007 L   000036 CALCH     0005     000000 COEF      0007     000001 CONVG
     0006     000625 CPW1      0006     000564 CPSUM     0006     000604 DATA      0005     005670 DELN      0010     000002 DEMAND
     0006     001167 DENS      0005 R   002734 EN        0004     000000 END       0005 R   005360 ENLN      0006 R   001263 ENLSAV
     0006 R   000000 ENN       0006 R   001261 ENNL      0006 R   001262 ENSAVE    0006     001073 ENTH      0006 R   000566 EQRAT
     0006     001112 FAZ       0000 R   000003 FCAL      0000 R   000012 FF        0000 R   000002 FHH       0006     001150 FOX
     0000 R   000001 FOO       0004     000001 GAS       0003     000001 GMET      0010     000000 GRAPH     0007     000003 HP
     0006 R   000572 HPP       0000 R   000011 HS        0006 R   000567 HSUB0     0005     005524 H0        0007 I   000030 IC
     0007     000000 IDEBUG    0004 I   000002 IE        0007     000015 IMAT      0000     000040 INJP$     0007 L   000023 IONS
     0007     000021 IP        0007 I   000037 IGSAVE    0007 I   000016 IQ1       0007 I   000005 ISV       0007     000034 IT
     0005 I   011444 IUSE      0004     000003 IZERO     0000 I   000005 J         0007 I   000026 JLIQ      0010 I   000001 JOUT
     0007 I   000025 JSOL      0007     000031 JS1       0007     000014 KMAT      0004 I   000004 LANK      0006 I   000463 LLMT
     0000 I   000004 LL1       0007 I   000040 LSAVE     0004     000005 MOL       0007     000006 MOLES     0006     000626 NAME
     0007     000024 NC        0007     000022 NEWR      0007     000035 NFZ       0007 I   000012 NLM       0007     000017 NOF
     0007     000020 NOMIT     0007     000007 NP        0007 I   000011 NPT       0007     000027 NREAC     0007 I   000013 NS
     0000 I   000000 NSPP1     0007     000010 NT        0006 R   000565 OF        0004     000006 OX        0006     001227 OXF
     0001     000002 PATM      0006     001054 PECWT     0006     000563 PP        0003 R   000003 RRAR      0003     000004 RRR
     0006 R   000574 RH        0006 R   001206 RHOP      0006     001207 RMW       0006     001131 RTEMP     0003     000005 RVR
     0005     002570 S         0007     000033 SHOCK     0005 R   011754 SLN       0007     000004 SP        0005     010770 SUB
     0000 R   000000 SUM       0006     000031 SUMN      0006     000003 SO        0005     011610 TEMP      0006     000547 THIGH
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 0005    001226 TLN        0006    000560 TLOW       0006    000557 TM         0006    000561 TMID       0007    000002 IP
 0006    000002 IT         0006 R  000576 VMIN       0007 L  000032 VOL        0006 R  000600 VPLS       0000 R  000010 VI
 0000 R  000007 V2         0006    000602 WP         0004    000007 ZERO


00101       1*           SUBROUTINE SAVE                                                                    000000
00101       2*     C                                                                                         000000
00101       3*     C   SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES                  000000
00101       4*     C                                                                                         000000
00103       5*           COMMON /CONSTS/ ATMN,GMET,PAIM,RBAR,RBR,RVR                           /CONSTS/     000000
00104       6*           COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                     /HOLCON/     000000
00104       7*     C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                    000000
00104       8*     C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                     000000
00105       9*           INCLUDE SPECPK                                                                     000000
00111      10*           COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),              /MISC/       000000
00111      11*          1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,         /MISC/       000000
00111      12*          2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),         /MISC/       000000
00111      13*          3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),      /MISC/       000000
00111      14*          4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,       /MISC/       000000
00111      15*          5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                  /MISC/       000000
00112      16*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,       /INDX/       000000
00112      17*          1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,      /INDX/       000000
00112      18*          2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE        /INDX/       000000
00112      19*     C                                                                                         000000
00113      20*              COMMON /CCC/ GRAPH,JOUT,DEMAND                                                   000000
00113      21*     C                                                                                         000000
00114      22*           DATA FUU/4HU, C/,FHH/4HH, C/,FCAL/4HAL/G/                                          000000
00120      23*           LOGICAL CALCH,IONS,VOL                                                             000000
00120      24*     C                                                                                         000000
00121      25*           IF(ISV)100,10,200                                                                  000000
00121      26*     C   NEXT POINT FIRST T IN SCHEDULE, USE PREVIOUS COMPOSITIONS FOR THIS T                 000000
00124      27*       10  IQ1 = IQSAVE                                                                       000003
00125      28*           ENN = ENSAVE                                                                       000005
00126      29*           ENNL = ENLSAV                                                                      000007
00127      30*           LLI = NLM                                                                          000011
00130      31*           DO 50 J = 1,NS                                                                     000042
00133      32*           IF (.NOT. IONS .OR. LLMT(NLM) .EQ. LSAVE)  GO TO 15                                000047
00135      33*           IF(LLMT(NLM).EQ.IE)  GO TO 13                                                      000043
00137      34*           IF(IUSE(J).NE.-10000)  GO TO 15                                                    000046
00141      35*           IUSE(J) = 0                                                                        000051
00142      36*           LLI  = NLM+1                                                                       000052
00143      37*           GO TO 20                                                                           000054
00144      38*        13 IF(SLN(J).NE.0..OR.IUSE(J).NE.0)  GO TO 15                                         000056
00146      39*           LLI = NLM-1                                                                        000065
00147      40*           IUSE(J) = -10000                                                                   000067
00150      41*           GO TO 50                                                                           000071
00151      42*        15 IF (IUSE(J).EQ.0) GO TO 20                                                         000073
00153      43*           EN (J,NPT) = SLN(J)                                                                000074
00154      44*           IF(IUSE(J).GT.0) IUSE(J) = - IUSE(J)                                               000076
00156      45*           IF (EN(J,NPT) .GT. 0.0)  IUSE(J) = - IUSE(J)                                       000133
00160      46*           GO TO 50                                                                           000110
00161      47*        20 EN(J,NPT) = 0.                                                                     000112
00162      48*           ENLN(J) = SLN(J)                                                                   000112
00163      49*           IF (ENLN(J) + 18.50 .LE. ENNL)  GO TO 50                                           000114
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00165            EN(J,NPT) = EXP(ENLN(J))                                                  000120
00166         50 CONTINUE                                                                  000131
00170            NLM = LL1                                                                 000131
00171            RETURN                                                                    000133
00171      C  FIRST T--SAVE COMPOSITIONS FOR FUTURE POINTS WITH THIS T                     000133
00172       100  ISV = -ISV                                                                000137
00173            IQSAVE = IQ1                                                              000140
00174            ENSAVE = ENN                                                              000142
00175            ENLSAV = ENNL                                                             000144
00176            LSAVE = LLMT(NLM)                                                         000146
00177            DO 150 J = 1,NS                                                           000161
00202            SLN(J) = ENLN(J)                                                          000161
00203       150  IF (IUSE(J) .NE. 0)  SLN(J) = EN(J,ISV)                                   000162
00203      C  USE COMPOSITIONS FROM PREVIOUS POINT                                         000162
00206       200  DO 300 J = 1,NS                                                           000172
00211       300  EN(J,NPT) = EN(J,ISV)                                                     000207
00213            RETURN                                                                    000211
00213      C  CALCULATE NEW VALUES OF BO AND HSUB0 FOR NEW OF RATIO                        000211
00214            ENTRY NEWOF                                                               000214
00215            WRITE(JOUT,730) OF                                                        000214
00220       730 FORMAT(6H0OF = ,F10.6)                                                     000222
00221            SUM = OF + 1.                                                             000222
00222            V2 =    (OF*VMIN(1)+VMIN(2))/SUM                                          000225
00223            V1 =    (OF*VPLS(1)+VPLS(2))/SUM                                          000232
00224            IF (V2 .LT. 0.0)  EQRAT = ABS(V1/V2)                                      000237
00226            IF (RH(1) .GT. 0.0 .AND. RH(2) .GT. 0.0)  GO TO 744                       000246
00230            RHOP = RH(2)                                                              000262
00231            IF (RHOP .LE. 0.0)  RHOP = RH(1)                                          000264
00233            GO TO 745                                                                 000271
00234       744 RHOP =  (OF+1.)*RH(1)*RH(2)/(RH(1)+ OF *RH(2))                             000273
00235       745  DO 747 J = 1,NLM                                                          000304
00240       747  BO(J) = (BOP(J,2) + BOP(J,1)*OF)/SUM                                      000310
00242            NPT = 1                                                         MAINU137  000315
00243            IF(.NOT.CALCH)  GO TO 750                                                 000317
00245            CALL HCALC                                                                000321
00246            CALCH = .FALSE.                                                           000323
00247            IF (OF .GT. 0.0)  HPP(1) = SUM*HPP(1)/OF                                  000324
00251            HPP(2) = SUM*HPP(2)                                                       000333
00252            GO TO 760                                                                 000336
00253       750  HSUB0 = (HPP(2) + HPP(1)*OF)/(RBAR*SUM)                                   000340
00254       760 IC = 0                                                                     000347
00255            JSOL = 0                                                                  000347
00256            JLIQ = 0                                                                  000350
00257            HS = RBAR*HSUB0                                                           000351
00260            WRITE(JOUT,773)                                                           000354
00262       773 FORMAT (1H0,17X,4HFUEL ,13X,7HOXIDANT  ,12X,7HMIXTURE    //)     MAINU124  000361
00263       780 FORMAT (1H 2A4,3E18.8/)                                           MAIN012  000361
00264            FF = FHH                                                                  000361
00265            IF(VOL)FF = FVV                                                           000363
00267            WRITE(JOUT,780) FF,FCAL ,HPP(2),HPP(1),HS                                 000367
00276            WRITE(JOUT,785)                                                           000403
00300       785 FORMAT (12H KG-ATOMS/KG)                                                   000410
00301            WRITE(JOUT,780) (LLMT(J),LANK,BOP(J,2),BOP(J,1),BO(J), J = 1,NLM)         000413
00313            RETURN                                                                    000426
00314            END                                                                       000470
END FO
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@FOR,S LEWIS.SEARCH,LEWIS.SEARCH
[illegible] -10/25/79-17:40:07 (9,)


   SUBROUTINE SEARCH     ENTRY POINT 000424


   STORAGE USED: CODE(1) 000440; DATA(0) 000114; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003     MOLCON 000010
    0004     SPECES 012120
    0005     MISC   001264
    0006     INDX   000041
    0007     CCC    000003


   EXTERNAL REFERENCES (BLOCK, NAME)

    0010     NRDU$
    0011     N102$
    0012     N101$
    0013     NWDU$
    0014     NERR3$


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

   0000     000022 10F        0001     000014 123G       0001     000015 126G       0001     000043 144G       0001     000303 145L
   0001     000075 152G       0001     000120 167G       0001     000306 170L       0001     000121 171G       0001     000321 171L
   0000     000045 172F       0000     000055 176F       0000     000030 20F        0001     000137 202G       0001     000147 205G
   0001     000177 216G       0001     000204 223G       0001     000215 231G       0001     000271 252G       0001     000341 275G
   0001     000371 304G       0000     000020 5F         0001     000035 7L         0001     000162 805L       0001     000164 810L
   0001     000220 820L       0001     000227 825L       0000     000032 871F       0004 R 006034 A          0005     000570 AM
   0005     000624 AM1        0005     000741 ANUM       0005     000004 ATOM       0000 R 000001 B          0005     000502 BO
   0005     000521 BOP        0006     000036 CALCH      0004 R 000000 COEF       0006     000001 CONVG      0005     000625 CPR1
   0005     000564 CPSUM      0005     000604 DATA       0004 R 002734 DATE       0004     005670 DELN       0007     000002 DEMAND
   0005     001167 DENS       0004     002734 EN         0003 I 000000 END        0004     005360 ENLN       0005     001263 ENLSAV
   0005     000000 ENN        0005     001261 ENNL       0005     001262 ENSAVE     0005     001073 ENTH       0005     000566 EQRAT
   0005     001112 FAZ        0005     001150 FOX        0003 I 000001 GAS        0007     000000 GRAPH      0006     000003 HP
   0005     000572 HPP        0005     000567 HSUBO      0004     005524 HO         0000 I 000013 I          0006     000030 IC
   0006     000000 IDEBUG     0003     000002 IE         0006     000015 IMAT       0000     000066 INJP$      0006     000023 IONS
   0006     000021 IP         0006     000037 IQSAVE     0006     000016 IQ1        0006     000005 ISV        0006     000034 IT
   0004 I 011444 IUSE       0000 I 000012 IX         0003     000003 IZERO      0000 I 000014 J          0006     000026 JLIQ
   0007 I 000001 JOUT       0006     000025 JSOL       0006     000031 JS1        0000 I 000017 K          0006     000014 KMAT
   0006 I 000012 L          0003     000004 LANK       0005 I 000463 LLMT       0006     000040 LSAVE      0003     000005 MOL
   0006     000006 MOLES      0000 I 000005 MT         0005     000626 NAME       0006 I 000024 NC         0006 L 000022 NEWR
   0006     000035 NFZ        0006     000017 NOF        0006 I 000020 NOMIT      0006     000007 NP         0006     000011 NPT
   0006     000027 NREAC      0006 I 000013 NS         0000 I 000000 NSPP1      0006     000010 NT         0005     000565 OF
   0004 I 005360 OMIT       0003     000006 OX         0005     001227 OXF        0005     001054 PECWT      0000 I 000011 PHAZ
   0005     000563 PP         0005     000574 RH         0005     001206 RHOP       0005     001207 RMW        0005     001131 RTEMP
   0004     002570 S          0006     000033 SHOCK      0004     011754 SLN        0006     000004 SP         0004 I 010770 SUB
   0005     000001 SUMN       0005     000003 SO         0004 R 011610 TEMP       0005 R 000562 THIGH      0005     001226 TLN
   0005 R 000560 TLOW       0005     000557 TM         0005 R 000561 TMID       0006     000002 TP         0005     000002 TT
   0000 R 000015 T1         0000 R 000016 T2         0005     000576 VMIN       0006     000032 VOL        0005     000600 VPLS
```

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```
0005    000602 *P         0003    000007 ZERO


00101              SUBROUTINE SEARCH                                                              000000
00101         C                                                                                   000000
00101         C  SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED                         000000
00101         C                                                                                   000000
00103              COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                   /HOLCON/   000000
00103         C    COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                000000
00103         C   1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                 000000
00104                 INCLUDE SPECPK                                                              000000
00110              COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),           /MISC/     000000
00110             1               BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,      /MISC/     000000
00110             2               HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),      /MISC/     000000
00110             3               DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),   /MISC/     000000
00110             4               ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,    /MISC/     000000
00110             5               RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV               /MISC/     000000
00111              COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,       /INDX/     000000
00111             1               KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,   /INDX/     000000
00111             2               NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE     /INDX/     000000
00111         C                                                                                   000000
00112                 COMMON /CCC/ GRAPH,JOUT,DEMAND                                              000000
00112         C                                                                                   000000
00113              DIMENSION B(4),DATE(2,3),MT(4),OMIT(3,3)                                       000000
00114              EQUIVALENCE (DATE,EN),(ENLN,OMIT)                                              000000
00115              INTEGER END,GAS,OMIT,PHAZ,SUB                                                  000000
00116              LOGICAL NEWR                                                                   000000
00116         C                                                                                   000000
00117              NC= 0                                                                          000000
00120              IX= 0                                                                          000000
00121              SUB(1,1) = END                                                                 000001
00122              DO 3 I=1,150                                                                   000015
00125              DO 3  J=1,L                                                                    000015
00130        3     A(J,I) = 0.0                                                                   000015
00133              READ(4,5)  TLOW,TMID,THIGH                                                     000022
00140          5 FORMAT (3F10.3)                                                                  000032
00141              NS = 1                                                                         000032
00142          7 READ     (4,10)(SUB(NS,I),I=1,3),DATE(1,NS),DATE(2,NS),(MT(J),B(J),              000035
00142           1  J=1,4),PHAZ,T1,T2                                                              000035
00162         10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3)                                          000105
00163              IF(SUB(NS,1).EQ.END) GO TO 171                                                 000105
00165              READ     (4,20) ((COEF(I,J,NS),J=1,7),I=1,2)                                   000110
00176         20 FORMAT (5E15.8)                                                                  000130
00177              IF(NOMIT.EQ.0) GO TO 810                                                       000130
00201              DO 805 I=1,NOMIT                                                               000132
00204              DO 804 J=1,3                                                                   000147
00207      804   IF (OMIT(J,I) .NE. SUB(NS,J))  GO TO 805                                         000147
00212              GO TO 7                                                                        000160
00213       805 CONTINUE                                                                          000164
00215       810 DO 820 K=1,4                                                                      000164
00220              IF(B(K).EQ.0.) GO TO 825                                                       000177
00222              DO 168 I=1,L                                                                   000204
00225      168   IF (LLMT(I) .EQ. MT(K))  GO TO 820                                               000204
00230              DO 819 J=1,L                                                                   000215
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00233      52*         819 A(J,NS) = 0.                                                           000215
00235      53*             GO TO 7                                                                000216
00236      54*         820 A(I,NS)= B(K)                                                          000220
00240      55*         825 IUSE(NS) = 0                                                           000227
00241      56*             IF(PHAZ.EQ.GAS) GO TO 170                                              000230
00243      57*             NC= NC+1                                                               000233
00244      58*             TEMP(NC,1)= T1                                                         000236
00245      59*             TEMP(NC,2)= T2                                                         000241
00246      60*             IX= IX+1                                                               000243
00247      61*             IF((IUSE(NS-1).EQ.0 .OR. NC.EQ.1) GO TO 145                            000246
00251      62*             DO 830 I=1,L                                                           000271
00254      63*        830  IF (A(I,NS) .NE. A(I,NS-1))  GO TO 145                                 000271
00257      64*             IX= IX-1                                                               000277
00260      65*         145 IUSE(NS)= -IX                                                          000303
00261      66*         170 NS= NS+1                                                               000306
00262      67*             IF (NS .LT. NSPP1)  GO TO 7                                            000310
00264      68*             WRITE (JOUT,871)                                                       000313
00266      69*        871  FORMAT (//20X,54HDIMENSIONS IN /SPECES/ FOUND TO BE TOO SMALL IN S     000321
00266      70*            1EARCH/)                                                                000321
00267      71*         171 NS= NS-1                                                               000321
00270      72*             NEWR= .FALSE.                                                          000323
00271      73*             WRITE(JOUT,172)                                                        000330
00273      74*         172 FORMAT(42H0SPECIES BEING CONSIDERED IN THIS SYSTEM    )                000341
00274      75*             DO 174 I=1,NS,5                                                        000341
00277      76*             K = I + 4                                                              000344
00300      77*             IF (NS .LT. K)  K = NS                                                 000347
00302      78*        174  WRITE(JOUT,176)(DATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),        000355
00302      79*            1    J=I,K)                                                             000355
00315      80*         176 FORMAT(5(5X,2A3,2X,3A4))                                               000402
00316      81*             RETURN                                                                 000402
00317      82*             END                                                                    000437
END FOR
```

```
@FOR,S LEWIS.SHCK,LEWIS.SHCK
 SA  E  -10/25/79-17:40:16 (10,)

   SUBROUTINE SHCK       ENTRY POINT 001367

   STORAGE USED: CODE(1) 001401; DATA(0) 000263; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSTS 000006
    0004    HOLLON 000010
    0005    POINTS 000335
    0006    SPECES 012120
    0007    MISC   001264
    0010    DOUBLE 001560
    0011    INDX   000041
    0012    PERF   000166
    0013    OUPT   000073
    0014    CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0015    KDYES
    0016    PAGIT
    0017    CHRSIZ
    0020    GOUT
    0021    NEWOF
    0022    HCALC
    0023    OUT1
    0024    OUT2
    0025    EQLBRM
    0026    SAVE
    0027    OUT3
    0030    NWNL$
    0031    NRNL$
    0032    NWDU$
    0033    NIO2$
    0034    SQRT
    0035    NIO3$
    0036    NIO1$
    0037    ALOG
    0040    EXP
    0041    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000    000143 125F        0001    000211 14L         0001    000011 145G        0001    000221 15L         0001    001001 150L
    0000    000165 152F        0001    000222 156G        0000    000101 16F         0001    001112 161L        0001    000126 17L
    0001    000143 19L         0001    000073 204G        0001    000114 21L         0001    000136 223G        0001    000147 231G
    0001    000245 30L         0001    000356 323G        0001    000376 334G        0001    000520 361G        0001    000534 40L
    0001    001125 431L        0001    000320 44L         0001    000325 45L         0000    000137 46F         0001    001057 461G
    0001    000412 47L         0001    000547 50L         0001    001201 520G        0001    001232 536G        0001    001247 547G
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0001     001276 561G      0001     001303 572G      0000     000176 58F       0001     001322 604G      0001     001345 620G
0000     000122 68F       0001     000750 75L       0000     000111 861F      0000     000122 862F      0000     000131 863F
0001     001106 850L      0006     006034 A         0007     000570 AM        0007 R   000624 AM1       0007     000741 ANUM
0003     000000 ATMN      0007     000004 ATOM      0000 R   000036 AX        0000 R   000037 AXX       0000 R   000024 AI
0007     000502 BP        0007     000521 BOP       0011     000036 CALCH     0006     000000 COEF      0011     000001 CONVG
0005 R   000032 CPR       0007 R   000625 CPR1      0007     000564 CPSUM     0007     000604 DATA      0006     005670 DELN
0014     000002 DEMAND    0007     001167 DENS      0005 R   000064 DLVPT     0005 R   000047 DLVTP     0006 R   002734 EN
0004     000000 END       0006 R   005360 ENLN      0007     001263 ENLSAV    0007     000000 ENN       0007     001261 ENNL
0007     001262 ENSAVE    0007     001073 ENTH      0012 L   000165 EQL       0007     000566 EQRAT     0013     000002 FA
0013     000003 FAP       0007     001112 FAZ       0013 R   000005 FB        0013     000006 FC        0013     000007 FCP
0013     000012 FCST      0013     000014 FCV       0013     000015 FG        0013     000017 FGE       0013     000020 FGV
0013     000021 FH        0013     000023 FI        0013     000025 FIV       0013     000027 FM        0000 R   000001 FMM
0013 R   000031 FMT       0013 R   000050 FN        0013 R   000052 FOUR      0007     001150 FOX       0013     000053 FP
0000 R   000002 FFP       0000 R   000003 FRA       0000 R   000004 FRB       0013     000054 FS        0013     000056 FSV
0013     000057 FT        0013     000061 FTK       0000 R   000005 FT1       0000 R   000006 FU1       0000 R   000007 FU2
0013     000063 FV        0013 R   000065 FVEL      0000 R   000010 FV21      0000 R   000011 FV22      0000 R   000012 FV23
0013 R   000001 F13       0013     000000 F9X       0010 D   000000 G         0005 R   000101 GAMMAS    0000 R   000020 GAMMAI
0004     000001 GAS       0010 D   001516 GG        0003     000001 GMET      0014     000000 GRAPH     0011     000003 HP
0007     000572 HFP       0000 R   000030 HS        0007 R   000567 HSUBO     0005 R   000000 HSUM      0006     005524 HO
0000 I   000022 I         0011     000030 IC        0011 I   000000 IDEBUG    0004     000002 IE        0011     000015 IMAT
0000 L   000013 INCDEG    0000 L   000014 INCDFZ    0000     000233 INJPS     0000 I   000021 IOF       0011     000023 IONS
0011     000021 IF        0011     000037 IQSAVE    0011     000016 IQI       0011 I   000005 ISV       0011     000034 IT
0006 I   011444 IUSE      0004 I   000003 IZERO     0000 I   000025 J         0011     000026 JLIQ      0014 I   000001 JOUT
0011     000025 JSOL      0011     000031 JS1       0000 I   000040 K         0011     000014 KMAT      0004     000004 LANK
0007     000463 LIMT      0011     000040 LSAVE     0012 R   000116 MACHI     0004     000005 MOL       0011     000006 MOLES
0000 R   000017 MU12R1    0000 R   000016 MI        0012 R   000150 M2MI      0007 I   000626 NAME      0011     000024 NC
0011     000022 NEWB      0011     000035 NFZ       0011     000012 NLM       0011 I   000017 NOF       0011     000020 NOMIT
0011     000007 NP        0011 I   000011 NPT       0011 I   000027 NREAC     0011 I   000013 NS        0000 I   000023 NSK
0000 I   000000 NSPP1     0011     000010 NT        0007 R   000565 OF        0013     000067 ONE       0004     000006 OX
0007 R   001227 OXF       0005 R   000116 P         0003     000002 PATM      0012 R   000000 PCP       0007     001054 PECWT
0007 R   000563 PP        0005 R   000217 PPP       0000 R   000026 PI        0000 R   000031 P21       0000 R   000033 P21L
0003     000003 RBAR      0003 R   000004 RBR       0015 L   000000 RDVES     0007     000574 RH        0007     001206 RHOP
0000 R   000035 RHO12     0007     001207 RMW       0012 R   000133 RRHO      0007 R   001131 RTEMP     0003     000005 RVR
0006     002570 S         0000 L   000015 SEQL      0000     000041 SHKINP    0011     000033 SHOCK     0006     011754 SEN
0005     000251 SONVEL    0011     000004 SP        0005 R   000015 SSUM      0006     010770 SUB       0007     000001 SUMN
0007     000003 SO        0005 R   000150 T         0006     011610 TEMP      0007     000562 THIGH     0013 R   000070 THREL
0007 R   001226 TEN       0007     000560 TLOW      0007     000557 TM        0007     000561 TMID      0005     000320 TOTN
0011 L   000002 TF        0007 R   000002 TT        0005 R   000266 TTT       0013 R   000071 TWO       0000 R   000027 TI
0012 R   000047 T211      0000 R   000032 T21       0000 R   000034 T21L      0005 R   000303 UTWO      0012 R   000101 UI
0012 R   000064 U102      0005     000202 V         0007     000576 VMIN      0012     000032 VMOC      0011     000032 VOL
0007     000600 VPLS      0005 R   000234 WM        0007     000602 WP        0010 D   001510 X         0004     000007 ZERO
0013     000072 ZEROF
```

```
00101       1*           SUBROUTINE SHCK                                                               000000
00101       2*      C                                                                                  000000
00103       3*           COMMON /CONSIS/ ATMN,GMET,PATM,RBAR,RBR,RVR                      /CONSIS/     000000
00104       4*           COMMON /MOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                /MOLCON/     000000
00105       5*           COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                   000000
00105       6*          1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)              000000
00105       7*          . ,UTWO(13),TOTN(13)                                                           000000
00105       8*      .    COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)               000000
00105       9*      C   1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SEN(150)                000000
00106      10*           INCLUDE SPECEX                                                                000037
```

```
      COMMON /MISC/ ENN,SUMN,TT,SD,ATOM(3,101),LLMT(15),BO(15),          /MISC/      000000
     1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,      /MISC/      000000
     2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),      /MISC/      000000
     3              DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),   /MISC/      000000
     4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,    /MISC/      000000
     5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV               /MISC/      000000
      COMMON /DOUBLE/ G(20,21), X(20)                                                000000
      COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/      000000
     1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,   /INDX/      000000
     2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE     /INDX/      000000
      COMMON /PERF/ PCP(26),VMOC(13),T2T1(13),U1U2(13),U1(13),           /PERF/      000000
     1              MACH1(13),RRHO(13),M2M1(13),EQL                      /PERF/      000000
      COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),    /OUPT/      000000
     1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/      000000
     2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/      000000
     3              TWO,ZEROF                                            /OUPT/      000000
C                                                                                    000000
         COMMON /CCC/ GRAPH,JOUT,DEMAND                                              000000
C                                                                                    000000
      DATA FMM/6HM2/M1 /,FPP/6HP2/P1 /,FRA/6HRHO2/R/,FRB/6HHO1    /,                 000000
     1     FTT/6HP2/P1 /,FU1/6HU1  VE/,FU2/6HU2  VE/,FV21/6HV2(U1-/,                 000000
     2     FV22/6HU2/M/S/,FV23/2HEC/                                                 000000
      DOUBLE PRECISION G,GG,X                                                        000000
      EQUIVALENCE (X(4),GG)                                                          000000
      LOGICAL EQL,INCDEQ,INCDFZ,SEQL,TP                                              000000
C                                                                                    000000
         LOGICAL RDYES                                                               000000
C                                                                                    000000
      REAL M1,MACH1,M2M1,MU12RT                                                      000000
C                                                                                    000000
      NAMELIST /SHKINP/ GAMMA1,INCDEQ,INCDFZ,MACH1,U1                   /SHKINP/     000000
C                                                                                    000000
      IOF = 0                                                                        000000
      TP=.TRUE.                                                                      000000
      CPR1 = 0.                                                                      000007
      DO 10 I=1,13                                                                   000011
      MACH1(I)=0.                                                                    000011
   10 U1(I) = 0.0                                                                    000011
      GAMMA1 = 0.                                                                    000013
      INCDEQ = .TRUE.                                                                000014
      INCDFZ = .TRUE.                                                                000016
      DO 18 I = 1,NREAC                                                              000022
   18 NAME(I,5) = IZERO                                                              000022
         CALL PAGIT                                                                  000024
         CALL CHRSIZ(1)                                                              000026
         IF(RDYES('TYPE YES FOR PRESENT VALUES OF SHKINP NAMELIST',46))              000031
     1   WRITE(6,SHKINP)                                                             000031
         CALL CHRSIZ(4)                                                              000042
         CALL GOUT('TYPE NAMELIST  SHKINP HERE',21)                                  000045
      READ (5,SHKINP)                                                                000051
      WRITE(JOUT,SHKINP)                                                             000055
      SEQL = INCDEQ                                                                  000061
      IF (T(1) .LE. 0.0)  T(1) = RTEMP(1)                                            000063
      DO 20 I = 1,13                                                                 000073
      IF (MACH1(I) .LE. 0.0 .AND. U1(I) .LE. 0.0)  GO TO 21                          000073
   [illegible]  NSP = I                                                              000107
```

```
00212      21 IOF = IOF+1                                                       000114
00213         OF = OXF(IOF)                                                     000117
00214         CALL NEWOF                                                        000121
00215         INCDEQ = SEQL                                                     000123
00216      17 PP = P(1)                                                         000125
00217         TT = T(1)                                                         000127
00220         IF (INCDEQ) GO TO 19                                              000131
00220   C  FROZEN                                                               000131
00222         DO 118 I = 1,13                                                   000136
00225         DLVTP(I) = 1.0                                                    000136
00226   118   DLVPT(I) = -1.0                                                   000137
00230      19 DO 35  NPT=1,NSK                                                  000143
00233         PPP(NPT) = P(NPT)                                                 000147
00234         TTT(NPT) = T(NPT)                                                 000151
00235         IF(NPT.EQ.1)  GO TO 14                                            000153
00237         IF (PPP(NPT) .LE. 0.0)  PPP(NPT) = PPP(NPT-1)                     000156
00241         IF (TTT(NPT) .LE. 0.0)  TTT(NPT) = TTT(NPT-1)                     000163
00243         SSUM(NPT) = SSUM(NPT-1)                                           000170
00244         HSUM(NPT) = HSUM(NPT-1)                                           000172
00245         IF(           TTT(NPT).EQ.TT.AND.PPP(NPT).EQ.PP)  GO TO 15        000174
00247      14 PP = PPP(NPT)                                                     000211
00250         TT = TTT(NPT)                                                     000212
00251         CALL HCALC                                                        000214
00252         HSUM(NPT) = HSUBO                                                 000216
00253     15  IF (CPRI .GT. 0.0)  GAMMAI = CPRI/(CPRI - 1.0/AMI)                000221
00255         IF (GAMMAI .GT. 0.0)  GO TO 30                                    000231
00257         WRITE(JOUT,16)                                                    000234
00261     16  FORMAT (//20X,34HMISSING GAMMAI OR CP VALUE IN SHCK/)             000241
00262         RETURN                                                            000241
00263     30  AI = SQRT(RBR*GAMMAI*TT/AMI)                                      000245
00264         IF (UI(NPT) .LE. 0.0)  UI(NPT) = AI*MACHI(NPT)                    000255
00266         IF (MACHI(NPT) .LE. 0.0)  MACHI(NPT) = UI(NPT)/AI                 000263
00270         WM(NPT) = AMI                                                     000271
00271         CPR(NPT) = CPRI                                                   000273
00272     35  GAMMAS(NPT) = GAMMAI                                              000275
00274         EQL = .FALSE.                                                     000301
00274   C  OUTPUT--1ST CONDITION                                                000301
00275         WRITE(JOUT,861)                                                   000302
00277    861 FORMAT(1H1,43X,39HINCIDENT SHOCK WAVE PARAMETERS ASSUMING    )     000307
00300         IF(.NOT.INCDEQ)  GO TO 44                                         000307
00302                   WRITE(JOUT,862)                                         000311
00304    862 FORMAT (1H ,51X,23HEQUILIBRIUM COMPOSITION  //)                    000316
00305         GO TO 45                                                          000316
00306     44                  WRITE(JOUT,863)                                   000323
00310    863 FORMAT (1H ,53X,18HFROZEN COMPOSITION //)                          000325
00311     45 CALL OUT1                                                          000325
00312        WRITE(JOUT,46)                                                     000326
00314     46 FORMAT (16H INITIAL GAS (1) )                                      000336
00315        FMT(3) = F13                                                       000336
00316        FMT(4) = FOUR                                                      000340
00317        WRITE(JOUT,FMT) FN,FB,(MACHI(J), J = 1,NPT)                        000342
00327        FMT(4) = TWO                                                       000361
00330        WRITE(JOUT,FMT) FUI,FVEL,(UI(J), J = 1,NPT)                        000363
00340        CALL OUT2                                                          000401
00340   C      BEGIN CALCULATIONS FOR 2ND CONDITION                             000401
00341        IF(INCDEQ)   EQL = .TRUE.                                          000403
```

```
00343            NPT = 1                                                                    000407
00344         47 GAMMA1 = GAMMAS(NPT)                                                       000412
00345            M1 = WM(NPT)                                                               000414
00346            P1 = PPP(NPT)                                                              000416
00347            T1 = TTT(NPT)                                                              000420
00350            HS = HSUM(NPT)                                                             000422
00351            P21 = (2.*GAMMA1*MACH1(NPT)**2-GAMMA1+1.)/(GAMMA1+1.)                      000424
00352            T21 = P21*(2./MACH1(NPT)**2+GAMMA1-1.)/(GAMMA1+1.)                         000436
00353            IF((T1*T21).GT.2000..AND. EQL) T21 = .7*T21 + 600./T1                      000453
00355            MU12RT = AM1*U1(NPT)**2/(RBR*T1)                                           000473
00356            P21L=ALOG(P21)                                                             000503
00357            T21L=ALOG(T21)                                                             000507
00360            DO 100 I = 1,8                                                             000520
00363            TT=T21*T1                                                                  000520
00364            PP=P21*P1                                                                  000523
00365            IF (.NOT.EQL) GO TO 40                                                     000526
00367            CALL EQLBRM                                                                000530
00370            GO TO 50                                                                   000532
00370      C   FROZEN                                                                       000532
00371         40 TLN = ALOG (TT)                                                            000534
00372            CALL HCALC                                                                 000537
00373            HSUM(NPT) = HSUBO                                                          000542
00374            CPR(NPT) = CPR1                                                            000544
00375         50 RHO12 = M1*T21/(WM(NPT)*P21)                                               000547
00376            GG=RHO12*MU12RT                                                            000556
00377            G(1,1)=-GG*DLVPT(NPT)-P21                                                  000564
00400            G(1,2)=-GG*DLVTP(NPT)                                                      000572
00401            G(1,3)=P21-1.+MU12RT*(RHO12-1.)                                            000576
00402            GG = (U1(NPT)*RHO12)**2/RBR                                                000605
00403            G(2,1)=-GG*DLVPT(NPT)+TT*(DLVTP(NPT)-1.)/WM(NPT)                           000613
00404            G(2,2)=-GG*DLVTP(NPT)-TT*CPR(NPT)                                          000626
00405            G(2,3) = HSUM(NPT) - HS - U1(NPT)**2*(1.0 - RHO12**2)/(2.0*RBR)            000636
00406            X(3)=G(1,1)*G(2,2)-G(1,2)*G(2,1)                                           000652
00407            X(1)=(G(1,3)*G(2,2)-G(2,3)*G(1,2))/X(3)                                    000661
00410            X(2)=(G(1,1)*G(2,3)-G(2,1)*G(1,3))/X(3)                                    000671
00411            AX = X(1)                                                                  000701
00412            AXX = X(2)                                                                 000703
00413            IF(AX.LT.0.) AX = -AX                                                      000705
00415            IF (AXX.LT.0.) AXX = -AXX                                                  000712
00417            IF (AXX.GT.AX)  AX = AXX                                                   000717
00421            IF(AX.LT..00005)  GO TO 150                                                000725
00423            AX = AX/.4054652                                                           000731
00424            IF(AX.LE.1.)  GO TO 75                                                     000734
00426            X(1) = X(1)/AX                                                             000737
00427            X(2) = X(2)/AX                                                             000743
00430         75 P21L=P21L+X(1)                                                             000750
00431            T21L=T21L+X(2)                                                             000753
00432            P21=EXP(P21L)                                                              000757
00433        100 T21 = EXP(T21L)                                                            000763
00435            WRITE(JOUT,125) U1(NPT)                                                    000771
00440        125 FORMAT(25H0DID NOT CONVERGE FOR U1=,F8.2,66H   ANSWERS PROBABLY NO         001001
00440           1T RELIABLE, SOLUTION PROBABLY DOES NOT EXIST)                              001001
00441        150 RRHO(NPT) = 1./RHO12                                                       001001
00442            M2M1(NPT) = WM(NPT)/AM1                                                    001004
00443            PCP(NPT) = P21                                                             001007
00444            T2T1(NPT) = T21                                                            001013
```

```
00445     179*          IF (NPT .GE. IDEBUG .AND. IDEBUG .NE. 0) WRITE(JOUT,152) I,T21,P21         001013
00453     180*      152 FORMAT(10H0ITR NO.= ,I1,7X,7HT2/T1 =,F9.2,7X,7HP2/P1 =,F9.2 )             001036
00454     181*          UTWO(NPT) = U1(NPT)*RHO12                                                   001036
00455     182*          U1U2(NPT) = U1(NPT)-UTWO(NPT)                                               001042
00456     183*          IF(.NOT.EQL)  GO TO 161                                                     001044
00460     184*          DO 880 K=1,NS                                                               001057
00463     185*          IF(IUSL(K).LT.0)  GO TO 880                                                 001057
00465     186*          IF(ENLN(K).GT.-87..AND.ENLN(K).LT.87.) EN(K,NPT) = EXP(ENLN(K))             001061
00467     187*      880 CONTINUE                                                                    001110
00471     188*          GO TO 431                                                                   001110
00471     189*    C   FROZEN                                                                        001110
00472     190*      161 PPP(NPT) = PP                                                               001112
00473     191*          TTT(NPT) = TT                                                               001114
00474     192*          GAMMAS(NPT) = CPR(NPT)/(CPR(NPT) - 1.0/AM1)                                 001116
00475     193*      431 ISV = 0                                                                     001125
00476     194*          IF(NPT.LT.NSK)  ISV=NPT                                                     001125
00500     195*          IF(NPT.EQ.1)  ISV=-1                                                        001133
00502     196*          NPT = NPT+1                                                                 001140
00503     197*          IF(EQL)  CALL SAVE                                                          001143
00505     198*          IF(NPT.LE.NSK)  GO TO 47                                                    001147
00507     199*          NPT = NSK                                                                   001153
00507     200*    C   OUTPUT--2ND CONDITION                                                         001153
00510     201*          WRITE(JOUT,58)                                                              001155
00512     202*       58 FORMAT (16H0SHOCKED GAS (2) )                                               001162
00513     203*          FMT(4) = TWO                                                                001162
00514     204*          WRITE(JOUT,FMT) FU2,FVEL,(UTWO(J),J = 1,NPT)                                001164
00524     205*          CALL OUT2                                                                   001204
00525     206*          WRITE(JOUT,68)                                                              001206
00527     207*       68 FORMAT (26H0INCIDENT SHOCK PARAMETERS   )                                   001216
00530     208*          FMT(4) = THREE                                                              001216
00531     209*          WRITE(JOUT,FMT) FPP,FB,FB,(PCP(J), J = 1,NPT)                               001220
00542     210*          WRITE(JOUT,FMT) FTT,FB,FB,(T2T1(J), J = 1,NPT)                              001235
00553     211*          FMT(4) = FOUR                                                               001252
00554     212*          WRITE(JOUT,FMT) FMM,FB,FB,(M2M1(J), J = 1,NPT)                              001254
00565     213*          WRITE(JOUT,FMT) FRA,FRB,FB,(RRHO(J), J = 1,NPT)                             001271
00576     214*          FMT(4) = TWO                                                                001306
00577     215*          WRITE(JOUT,FMT) FV21,FV22,FV23,(U1U2(J), J = 1,NPT)                         001310
00610     216*          CALL OUT3                                                                   001325
00611     217*          INCDLC = .FALSE.                                                            001327
00612     218*          IF(INCDFZ.AND.EQL)  GO TO 17                                                001330
00614     219*          IF(IOF.LT.NOF)  GO TO 21                                                    001333
00616     220*          TP = .FALSE.                                                                001341
00617     221*          DO 999 K = 1,NREAC                                                          001345
00622     222*      999  RTEMP(K) = T(1)                                                            001345
00624     223*          RETURN                                                                      001347
00625     224*          END                                                                         001400
END FOR
```

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@FOR,S LEWIS.THERMP,LEWIS.THERMP
H.A  E3 -10/25/79-17:40:27 (8,)


   SUBROUTINE THERMP     ENTRY POINT 000376


   STORAGE USED: CODE(1) 000406; DATA(0) 000111; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSTS 000006
    0004    POINTS 000335
    0005    MISC   001264
    0006    INDX   000041
    0007    OUPT   000073
    0010    CCC    000003


   EXTERNAL REFERENCES (BLOCK, NAME)

    0011    NEWOF
    0012    ECL RM
    0013    OUT1
    0014    OUT2
    0015    OUT3
    0016    SAVE
    0017    NWDU$
    0020    NIO2$
    0021    NIO1$
    0022    NERR3$


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000     000017 10F        0000     000023 11F        0000     000031 12F        0001     000022 124G       0001     000044 131G
    0000     000037 20F        0000     000043 21F        0001     000220 217G       0000     000052 22F        0001     000245 233G
    0000     000004 5F         0001     000061 800L       0001     000111 860L       0001     000146 861L       0001     000173 862L
    0000     000060 863F       0001     000251 864L       0000     000066 868F       0001     000323 870L       0001     000352 871L
    0001     000006 95L        0005     000570 AM         0005     000624 AM1        0005     000741 ANUM       0003     000000 ATMN
    0005     000004 ATOM       0005     000502 BO         0005     000521 BOP        0006     000036 CALCH      0006     000001 CONVG
    0004     000032 CPR        0005     000625 CPR1       0005     000564 CPSUM      0005     000604 DATA       0010     000002 DEMAND
    0005     001167 DENS       0004     000064 DLVPT      0004     000047 DLVTP      0005     001263 ENLSAV     0005     000000 ENN
    0005     001261 ENNL       0005     001262 ENSAVE     0005     001073 ENTM       0005     000566 EQRAT      0007     000002 FA
    0007     000003 FAP        0005     001112 FAZ        0007 R   000005 FB         0007     000006 FC         0007     000007 FCP
    0007     000012 FCST       0007     000014 FCV        0007     000015 FG         0007     000017 FGE        0007     000020 FGV
    0007     000021 FH         0007     000023 FI         0007     000025 FIV        0007     000027 FM         0007 R   000031 FMT
    0007     000050 FN         0007     000052 FOUR       0005     001150 FOX        0007     000053 FP         0007     000054 FS
    0007     000056 FSV        0007     000057 FT         0007     000061 FTK        0000 R   000000 FUA        0000 R   000001 FUB
    0007     000063 FV         0007     000065 FVEL       0007     000001 F13        0007     000000 F9X        0004     000101 GAMMAS
    0013     000001 GMLT       0010     000000 GRAPH      0006 L   000003 HP         0005     000572 HPP        0005 R   000567 HSUBO
    0004     000000 HSUM       0000 I   000003 I          0006     000030 IC         0006 I   000000 IDEBUG     0006     000015 IMAT
    0000     000072 INJP$      0000 I   000002 IOF        0006     000023 IONS       0006 I   000021 IP         0006     000037 IOSAVE
    0006     000016 IOI        0006 I   000005 ISV        0006 I   000034 IT         0006     000026 JLIQ       0010 I   000001 JOUT
    0006     000025 JSNL       0006     000031 JSI        0006     000014 KMAT       0005     000463 LLMT       0006     000040 LSAVE
    0006     000006 MOLFS      0005     000626 NAME       0006     000024 NC         0006     000022 NEWR       0006     000035 NFZ
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0006     000012 NLM      0006 I 000017 NOF      0006     000020 NOMIT     0006 I 000007 NP     0006 I 000011 NPT
0006     000027 NREAC    0006   000013 NS       0006 I 000010 NT        0005 R 000565 OF     0007 R 000067 ONE
0005 R 001227 OXF        0004 R 000116 P        0003     000002 PATM      0005   001054 PECWT  0005 R 000563 PP
0004     000217 PPP      0003 R 000003 RBAR     0003     000004 RBR       0005   000574 RH     0005   001206 RHOP
0005     001207 RMW      0005   001131 RTEMP    0003     000005 RVR       0006   000033 SHOCK  0004   000251 SONVEL
0006 L 000004 SP         0004   000015 SSUM     0005     000001 SUMN      0005   000003 SO     0004 R 000150 T
0005     000562 THIGH    0007   000070 THREE    0005     001226 TLN       0005   000560 TLOW   0005   000557 TM
0005     000561 TMID     0004   000320 TOTN     0006 L 000002 TP        0005 R 000002 TT     0004   000266 TTT
0007 R 000071 TWO        0004 R 000202 V        0004 R 000303 VLM       0005   000576 VMIN   0006 L 000032 VOL
0005     000600 VPLS     0004   000234 WM       0005     000602 WP        0007   000072 ZERO
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```
00101      1*           SUBROUTINE THERMP                                                   000000
00101      2*     C                                                            MOLIU001     000000
00103      3*           COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                /CONSTS/     000000
00104      4*           COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)             000000
00104      5*          1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)        000000
00104      6*          2 ,VLM(13),TOTN(13)                                                      000000
00105      7*           COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),    /MISC/     000000
00105      8*          1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT, /MISC/     000000
00105      9*          2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2), /MISC/     000000
00105     10*          3              DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15), /MISC/  000000
00105     11*          4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,  /MISC/  000000
00105     12*          5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV           /MISC/    000000
00106     13*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,  /INDX/  000000
00106     14*          1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,VC,JSOL,JLIQ, /INDX/  000000
00106     15*          2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE   /INDX/  000000
00107     16*           COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),  /OUPT/  000000
00107     17*          1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/ 000000
00107     18*          2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,  /OUPT/  000000
00107     19*          3              TWO,ZERO                                          /OUPT/   000000
00107     20*     C                                                                             000000
00110     21*              COMMON /CCC/ GRAPH,JOUT,DEMAND                                       000000
00110     22*     C                                                                             000000
00111     23*           DATA FUA/6HU CAL//,FUB/6HGRAM  /                                        000000
00114     24*           LOGICAL HP,SP,TP,VOL                                                    000000
00114     25*     C                                                                             000000
00115     26*           IF (T(1) .LE. 0.0)  T(1) = 3800.0                                       000000
00117     27*           IOF = 0                                                                 000004
00120     28*        95 IOF = IOF+1                                                             000006
00121     29*           OF = OXF(IOF)                                                           000011
00122     30*           CALL NEWOF                                                              000013
00122     31*     C     SET ASSIGNED P OR VOLUME                                                000013
00123     32*           DO 871 IP = 1,NP                                                        000015
00126     33*           PP = P(IP)                                                              000035
00127     34*           VLM(NPT) = P(IP)                                                        000037
00127     35*     C     SET ASSIGNED T                                             MOLIU016     000037
00130     36*           DO 871 IT = 1,NT                                                        000044
00133     37*           TT = T(IT)                                                 MOLIU017     000044
00134     38*           CALL EQLBRM                                                MOLIU025     000046
00135     39*           IF (TT .GT. 0.0)  GO TO 800                                             000050
00137     40*           IF (NPT .EQ. 0)  RETURN                                                 000053
00141     41*       800 ISV = 0                                                                 000061
00142     42*           IF (IP .EQ. NP .AND. IT .EQ. NT .OR. TT .LE. 0.0)  GO TO 860            000061
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00144        ISV = NPT                                                                    000104
00145        IF(NPT.NE.13)  GO TO 870                                         MOLIU030   000104
00147    860 WRITE(JOUT,5)                                                                000111
00151      5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNEDMOLIU032   000115
00151       1)                                                                            000115
00152        IF(.NOT.VOL)  GO TO 861                                                      000115
00154        IF (HP)  WRITE(JOUT,10)                                                      000117
00157     10 FORMAT(1H0,62X,7H VOLUME /)                                                  000126
00160        IF (TP)  WRITE(JOUT,11)                                                      000126
00163     11 FORMAT(1H0,54X,22HTEMPERATURE AND VOLUME/)                                   000135
00164        IF (SP)  WRITE(JOUT,12)                                                      000135
00167     12 FORMAT(1H0,56X,18HENTROPY AND VOLUME/)                                       000144
00170        GO TO 862                                                                    000144
00171    861 IF(HP)  WRITE(JOUT,20)                                                       000146
00174     20 FORMAT(1H0,62X,10H PRESSURES  /)                                             000154
00175        IF(TP)  WRITE(JOUT,21)                                                       000154
00200     21 FORMAT(1H0,53X,24HTEMPERATURE AND PRESSURE/)                                 000163
00201        IF(SP)  WRITE(JOUT,22)                                                       000163
00204     22 FORMAT(1H0,55X,20HENTROPY AND PRESSURE/)                                     000173
00205    862 CALL OUT1                                                                    000173
00206        WRITE(JOUT,863)                                                              000174
00210    863 FORMAT (25H0THERMODYNAMIC PROPERTIES//)                                      000207
00211        IF(.NOT.VOL)  GO TO 864                                                      000207
00213        FMT(3) = ONE                                                                 000211
00214        IF (.NOT. HP)  GO TO 864                                                     000213
00216        DO 63 I=1,NPT                                                                000220
00221        FMT(I+2) = TWO                                                               000220
00222        IF (I .EQ. 13)  FMT(15) = 5HF9.2)                                            000222
00224    63  V(I) = RBAR*HSUBO                                                            000227
00226        WRITE(JOUT,FMT) FUA,FUB,FB,(V(I), I = 1,NPT)                                 000233
00237    864 CALL OUT2                                                                    000251
00240        CALL OUT3                                                                    000252
00241        IF (ISV .EQ. 0 .AND. IOF .EQ. NOF)  RETURN                                   000254
00243        IF(IDEBUG.GT.13)  IDEBUG=IDEBUG-13                                           000271
00245        WRITE(JOUT,868)                                                              000300
00247    868 FORMAT(1H1)                                                                  000305
00250        IF(NT.EQ.1.AND.NP.EQ.1)  GO TO 95                                            000305
00252        NPT = 0                                                                      000321
00253    870 NPT = NPT + 1                                                    MOLIU037   000323
00254        IF(.NOT.TP)  T(1)=TT                                                         000325
00256        IF(IP.EQ.1.AND.IT.EQ.1)  ISV=-ISV                                  12-22     000331
00260        IF(NT.EQ.1)  GO TO 871                                             12-22     000342
00262        IF(IT.EQ.NT)  ISV=0                                                          000345
00264    871 CALL SAVE                                                                    000352
00267        GO TO 95                                                                     000357
00270        END                                                              MOLIU045   000405
END FO
```

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@FOR,S LEWIS.VARFMT,LEWIS.VARFMT
H.A  E1S -10/25/79-17:40:34 (7,1)


   SUBROUTINE VARFMT     ENTRY POINT 000115


   STORAGE USED: CODE(1) 000124; DATA(0) 000023; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   OUPT    000073

   EXTERNAL REFERENCES (BLOCK, NAME)

    0004   NERR3$


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001     000006 114G        0001     000046 40L         0001     000100 45L         0003     000002 FA          0003     000003 FAP
    0003     000005 FB          0003     000006 FC          0003     000007 FCP         0003     000012 FCST        0003     000014 FCV
    0000 R   000000 FFOUR       0003     000015 FG          0003     000017 FGE         0003     000020 FGV         0003     000021 FH
    0003     000023 FI          0003     000025 FIV         0003     000027 FM          0003 R   000031 FMT         0003     000050 FN
    0000 R   000001 FONE        0003 R   000052 FOUR        0003     000053 FP          0003     000054 FS          0003     000056 FSV
    0003     000057 FT          0000 R   000002 FTHREE      0003     000061 FTK         0000 R   000003 FTWO        0003     000063 FV
    0003     000065 FVEL        0000 R   000004 FZERO       0003     000001 F13         0003     000000 F9X         0000 I   000005 I
    0000     000012 INJP$       0003 R   000067 ONE         0003 R   000070 THREE       0003 R   000071 TWO         0003 R   000072 ZERO


 00101      1*            SUBROUTINE VARFMT(V,NPT)                                                         000006
 00101      2*      C                                                                                      000006
 00103      3*            COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),       /OUPT/    000006
 00103      4*           1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR,  /OUPT/    000006
 00103      5*           2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,    /OUPT/    000006
 00103      6*           3              TWO,ZERO                                              /OUPT/    000006
 00103      7*      C                                                                                      000006
 00104      8*            DATA FFOUR/5HF9.4)/,FONE/5HF9.1)/,FTHREE/5HF9.3)/,FTWO/5HF9.2)/,                 000006
 00104      9*           1     FZERO/5HF9.0)/                                                              000006
 00112     10*            DIMENSION V(13)                                                                  000006
 00112     11*      C                                                                                      000006
 00113     12*            DO 45 I = 1,NPT                                                                  000006
 00116     13*            IF (I .GE. 13)  GO TO 40                                                         000006
 00120     14*            FMT(I+2) = FOUR                                                                  000012
 00121     15*            IF (V(I) .GE. 10.0)  FMT(I+2) = THREE                                            000014
 00123     16*            IF (V(I) .GE. 100.0)  FMT(I+2) = TWO                                             000022
 00125     17*            IF (V(I) .GE. 1.0E4)  FMT(I+2) = ONE                                             000030
 00127     18*            IF (V(I) .GE. 1.0E6)  FMT(I+2) = ZERO                                            000036
 00131     19*            GO TO 45                                                                         000044
 00132     20*         40 FMT(15) = FFOUR                                                                  000046
 00133     21*            IF (V(I) .GE. 10.0)  FMT(15) = FTHREE                                            000047
 00135     22*            IF (V(I) .GE. 100.0)  FMT(15) = FTWO                                             000055
 00137     23*            IF (V(I) .GE. 1.0E4)  FMT(15) = FONE                                             000063
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00141     24*          IF (V(I) .GE. 1.0E6)  FMT(15) = FZERO                          000071
00143     25*       45 CONTINUE                                                         000102
00145     26*          RETURN                                                           000102
00146     27*          END                                                              000123
END FOR

@BRKPT PRINT$
```

```
123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890**SEQ NO. 34







* * * * * *  UNIVAC 1100 TIME/SHARING EXEC  ACCOUNT NUMBER * 1HPD013K0000 VER. CR 33R3HOST1 SITE *  HOST 1   * * * * * *
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